



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 PM UTC

PDB ID : 2LLS / pdb\_00002lls  
BMRB ID : 18087  
Title : solution structure of human apo-S100A1 C85M  
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Deposited on : 2011-11-17

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

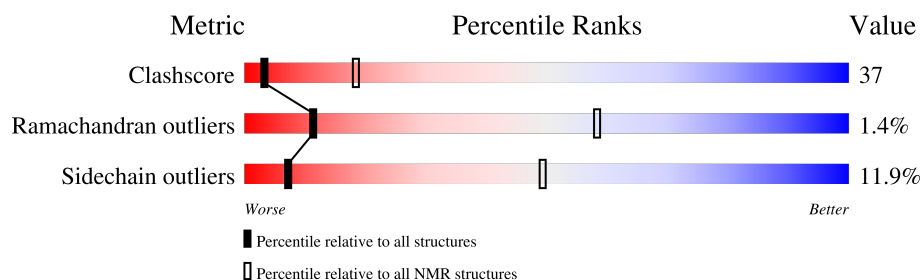
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 47%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 93     |                  |
| 1   | B     | 93     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:2-A:90, B:2-B:89 (177) | 0.88              | 11           |

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2888 atoms, of which 1420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A1.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 93       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1444  | 463 | 710 | 115 | 153 | 3 |       |
| 1   | B     | 93       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1444  | 463 | 710 | 115 | 153 | 3 |       |

There are 2 discrepancies between the modelled and reference sequences:

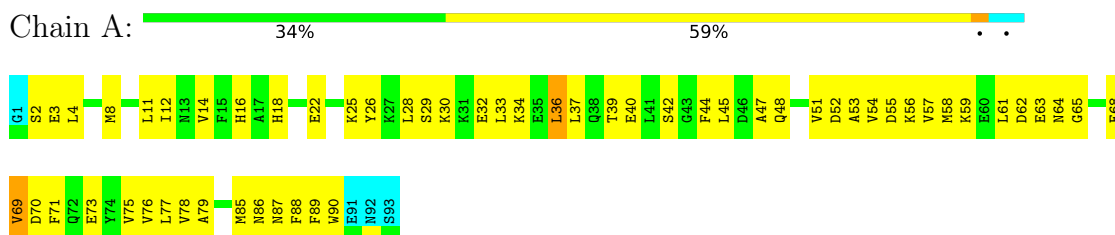
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 85      | MET      | CYS    | engineered mutation | UNP P23297 |
| B     | 85      | MET      | CYS    | engineered mutation | UNP P23297 |

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

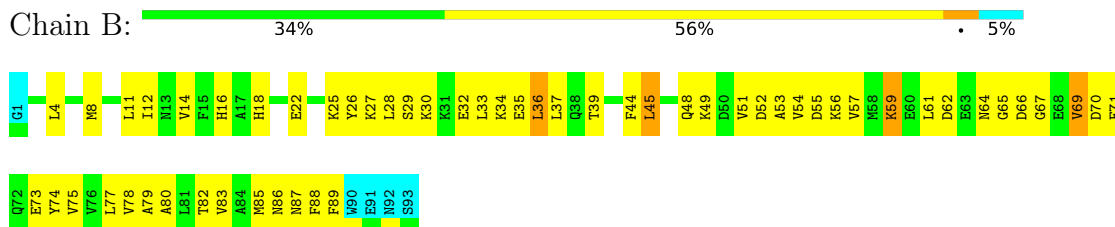
### 4.1 Average score per residue in the NMR ensemble

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

#### • Molecule 1: Protein S100-A1



#### • Molecule 1: Protein S100-A1

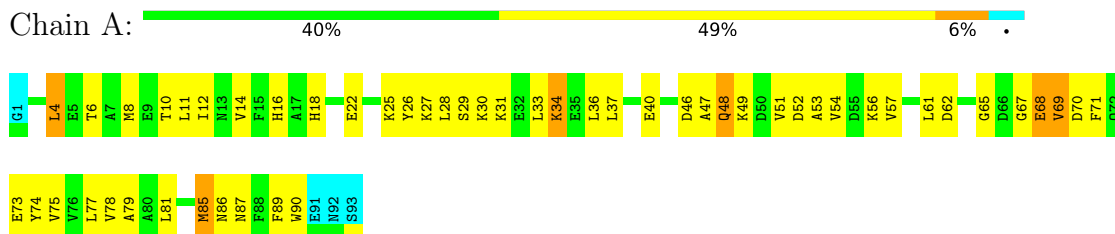


### 4.2 Scores per residue for each member of the ensemble

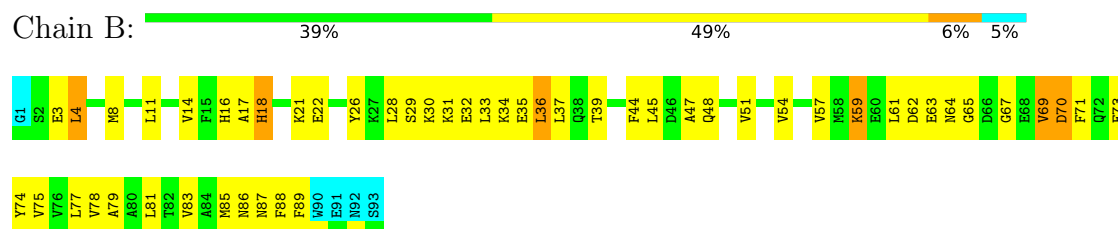
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

#### • Molecule 1: Protein S100-A1

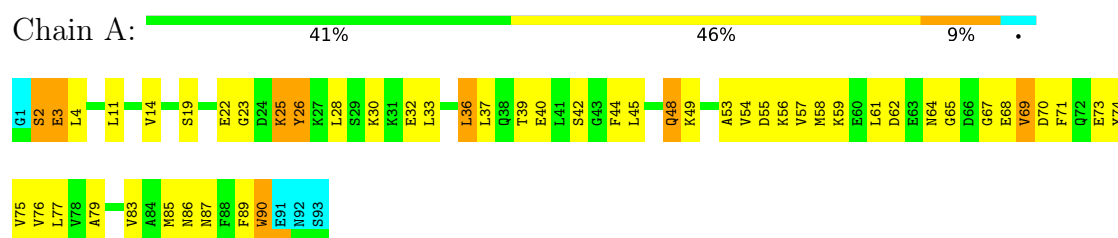


- Molecule 1: Protein S100-A1

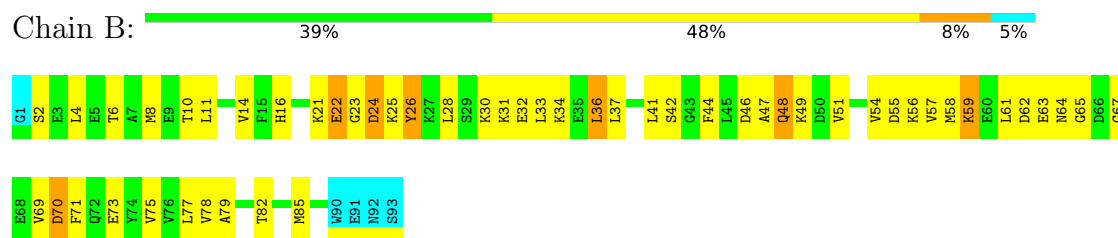


#### 4.2.2 Score per residue for model 2

- Molecule 1: Protein S100-A1

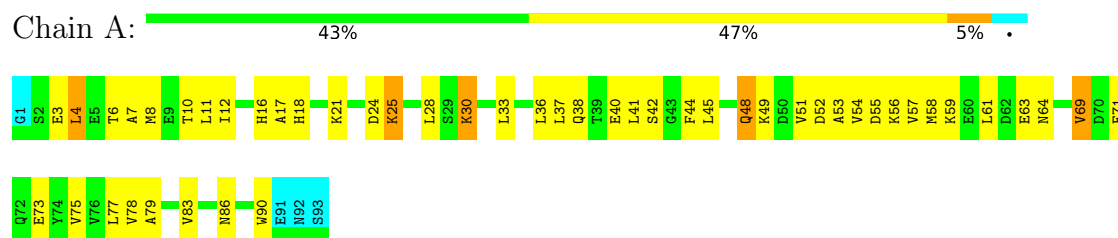


- Molecule 1: Protein S100-A1

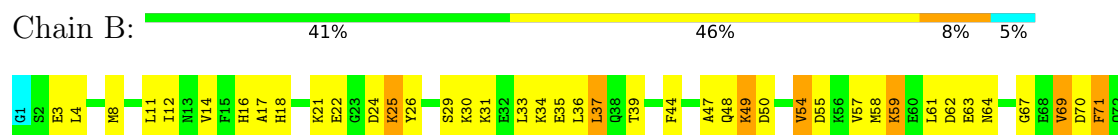


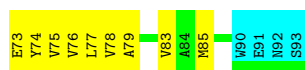
#### 4.2.3 Score per residue for model 3

- Molecule 1: Protein S100-A1



- Molecule 1: Protein S100-A1

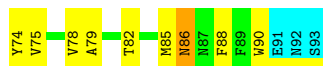




#### 4.2.4 Score per residue for model 4

- Molecule 1: Protein S100-A1

Chain A: 45% 41% 10% .



- Molecule 1: Protein S100-A1

Chain B: 32% 55% 8% 5%



#### 4.2.5 Score per residue for model 5

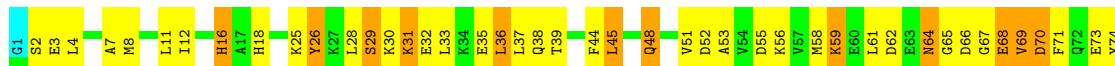
- Molecule 1: Protein S100-A1

Chain A: 31% 56% 9% .



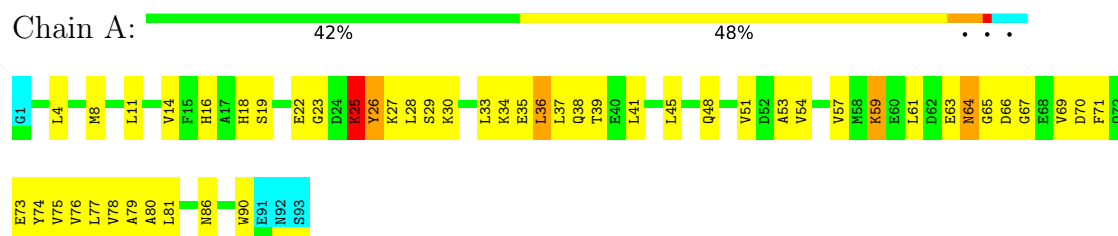
- Molecule 1: Protein S100-A1

Chain B: 33% 46% 15% 5%

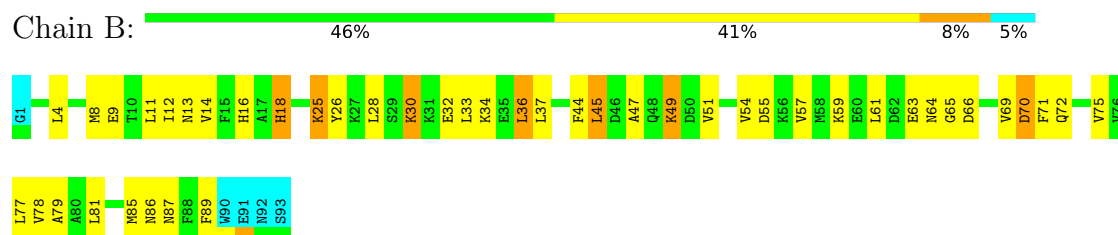


### 4.2.6 Score per residue for model 6

#### • Molecule 1: Protein S100-A1

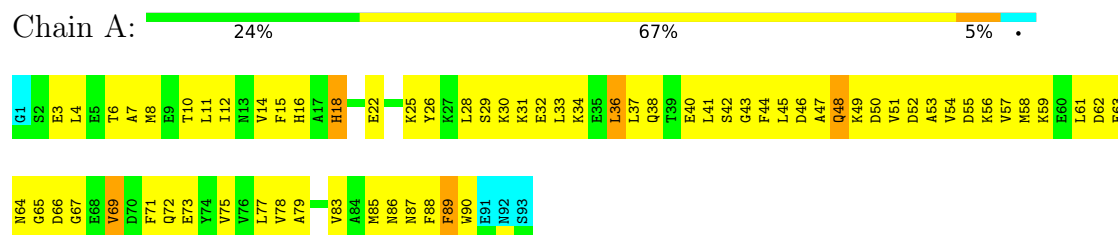


#### • Molecule 1: Protein S100-A1

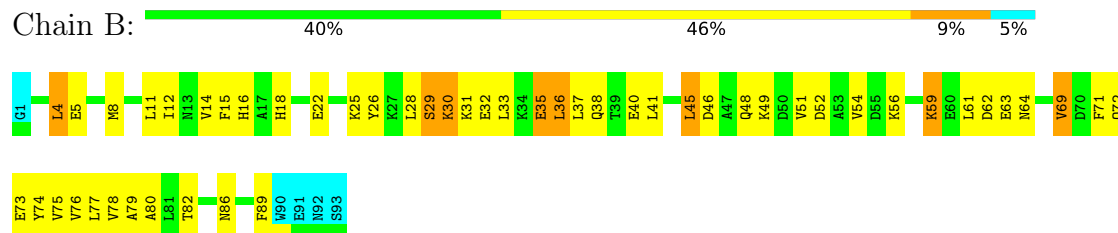


### 4.2.7 Score per residue for model 7

#### • Molecule 1: Protein S100-A1



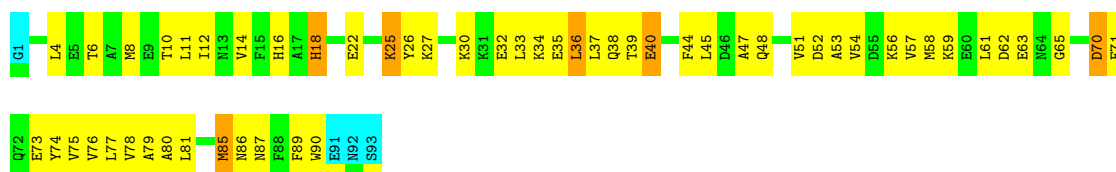
#### • Molecule 1: Protein S100-A1



### 4.2.8 Score per residue for model 8

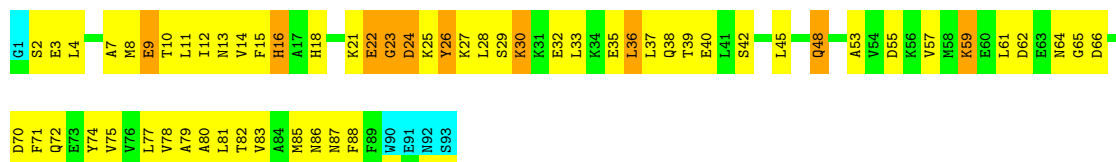
#### • Molecule 1: Protein S100-A1





• Molecule 1: Protein S100-A1

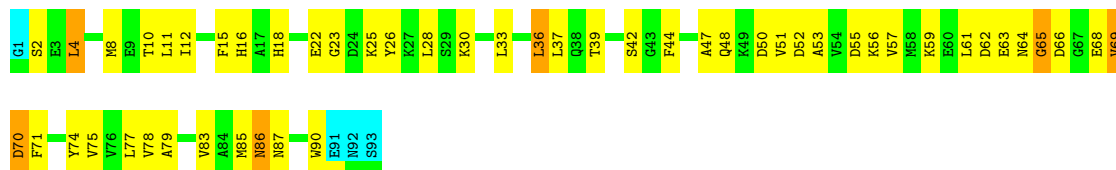
Chain B: 30% 54% 11% 5%



#### 4.2.9 Score per residue for model 9

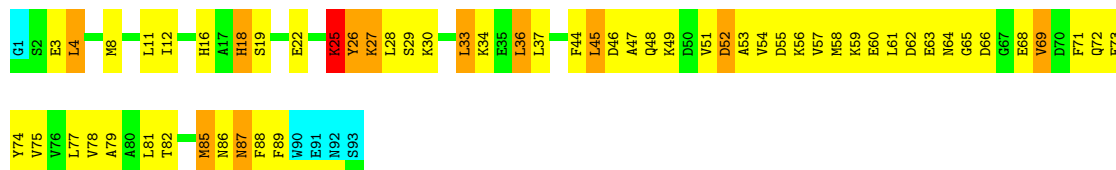
• Molecule 1: Protein S100-A1

Chain A: 41% 48% 6% 5%



• Molecule 1: Protein S100-A1

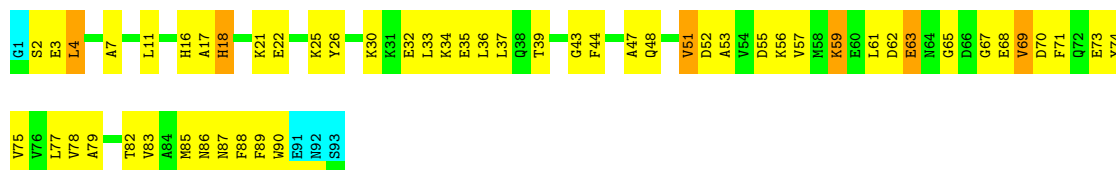
Chain B: 32% 49% 12% 5%



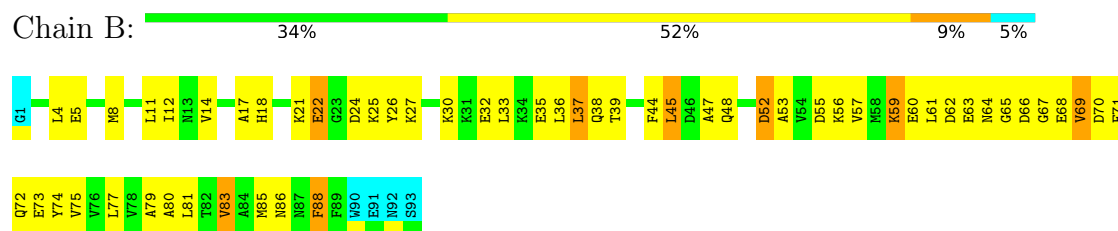
#### 4.2.10 Score per residue for model 10

• Molecule 1: Protein S100-A1

Chain A: 38% 52% 6% 5%

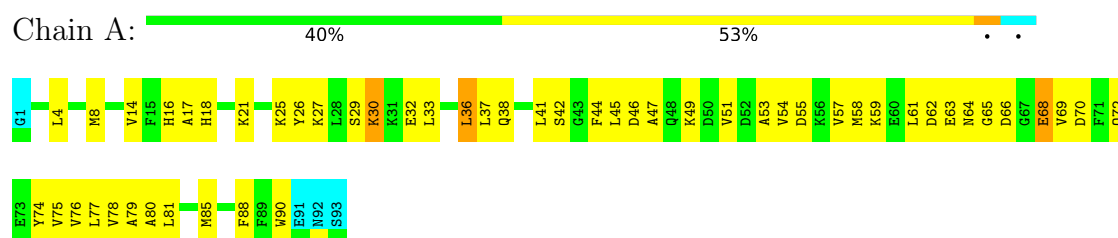


- Molecule 1: Protein S100-A1

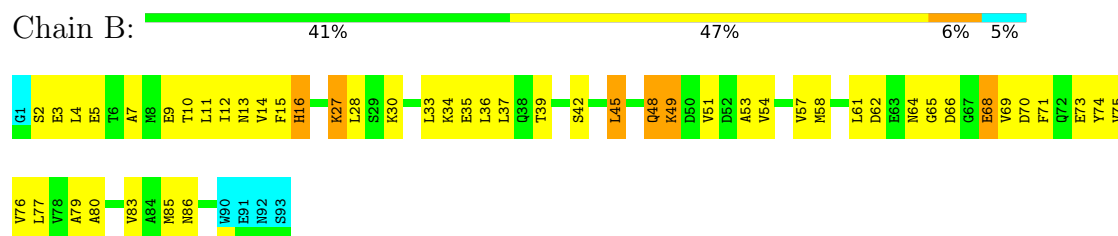


#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Protein S100-A1

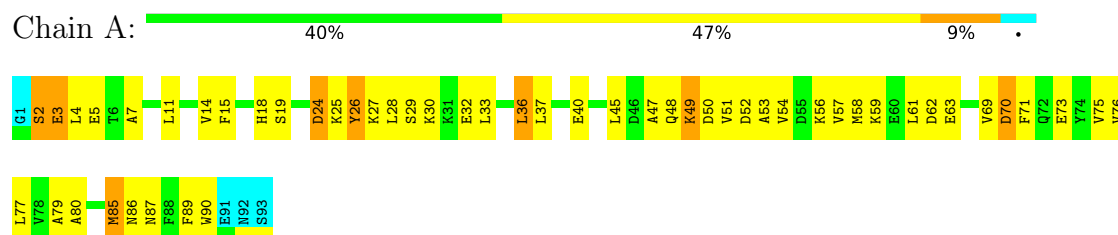


- Molecule 1: Protein S100-A1

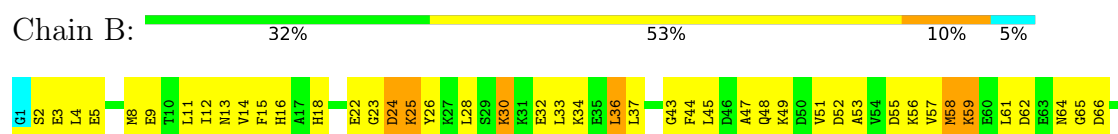


#### 4.2.12 Score per residue for model 12

- Molecule 1: Protein S100-A1



- Molecule 1: Protein S100-A1

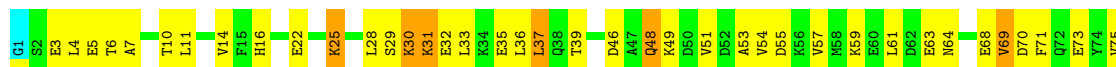




#### 4.2.13 Score per residue for model 13

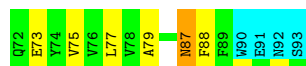
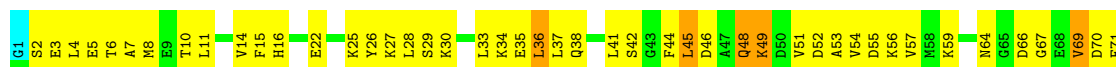
##### • Molecule 1: Protein S100-A1

Chain A: 47% 42% 6%



##### • Molecule 1: Protein S100-A1

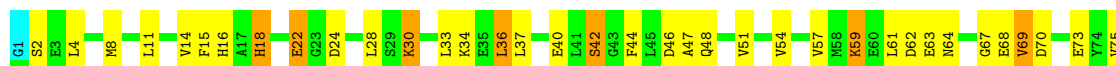
Chain B: 39% 49% 6% 5%



#### 4.2.14 Score per residue for model 14

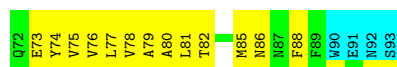
##### • Molecule 1: Protein S100-A1

Chain A: 46% 42% 8%



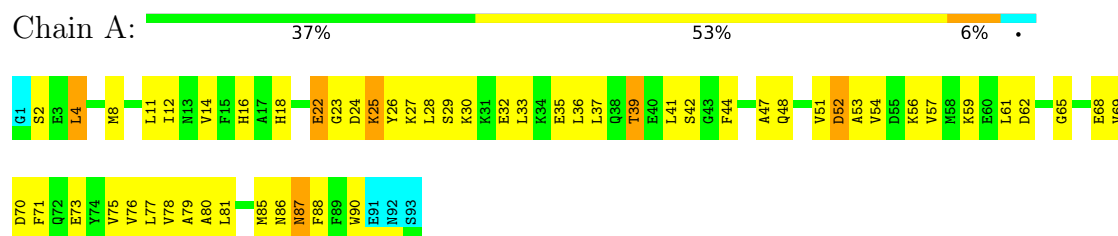
##### • Molecule 1: Protein S100-A1

Chain B: 37% 49% 9% 5%

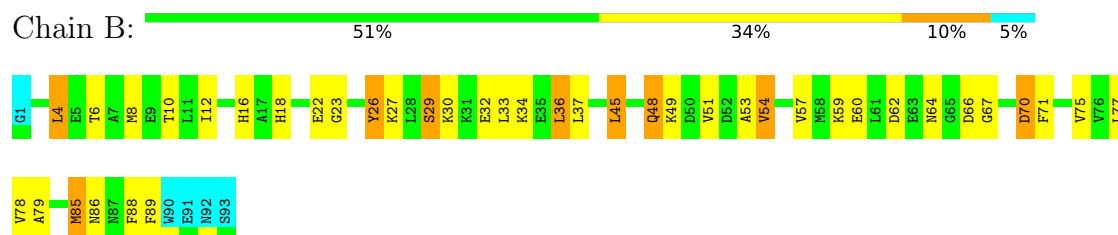


## 4.2.15 Score per residue for model 15

## • Molecule 1: Protein S100-A1

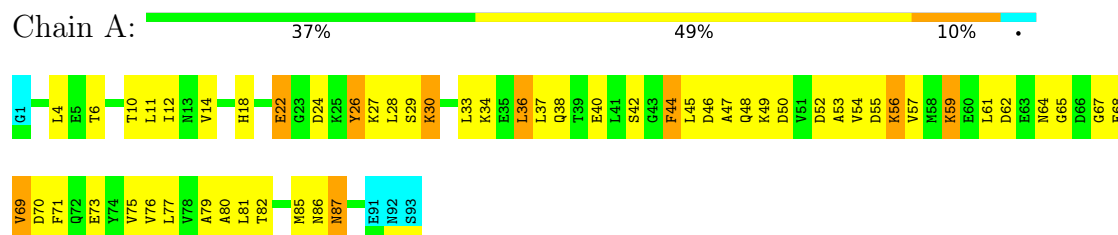


## • Molecule 1: Protein S100-A1

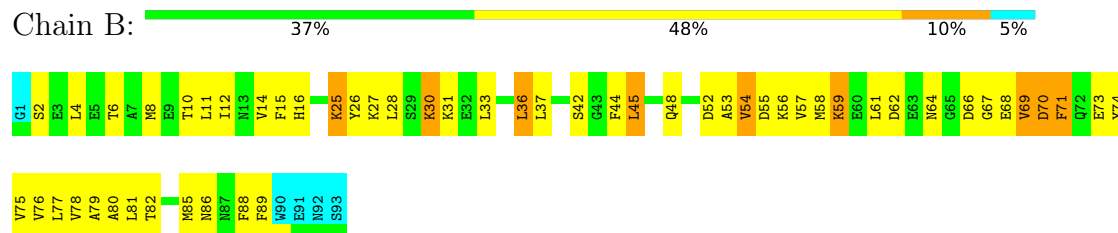


## 4.2.16 Score per residue for model 16

## • Molecule 1: Protein S100-A1



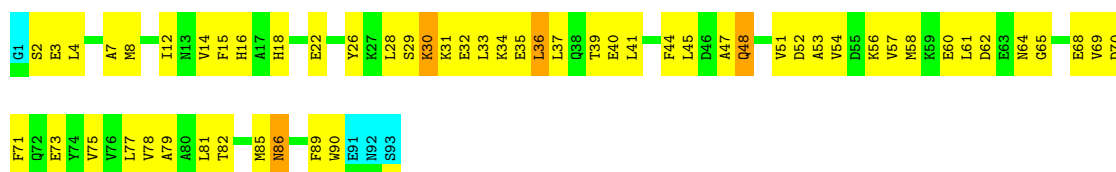
## • Molecule 1: Protein S100-A1



## 4.2.17 Score per residue for model 17

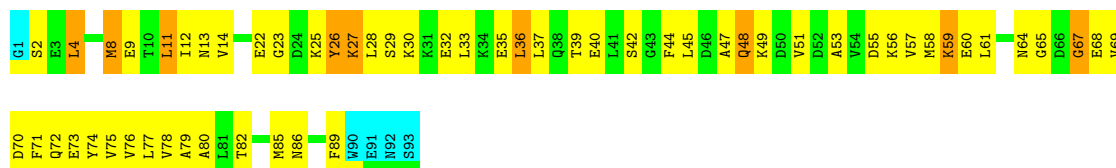
## • Molecule 1: Protein S100-A1





• Molecule 1: Protein S100-A1

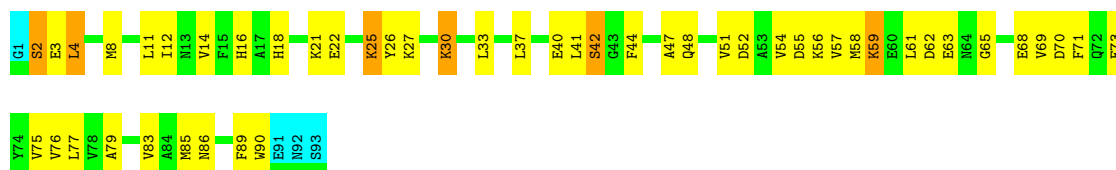
Chain B: 32% 53% 10% 5%



#### 4.2.18 Score per residue for model 18

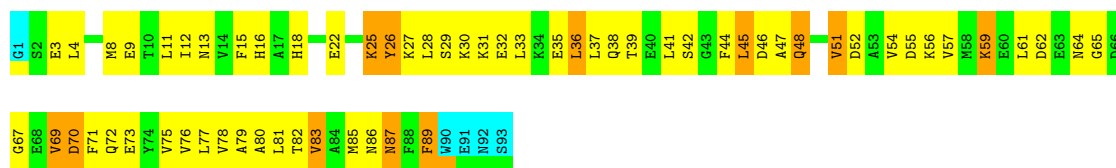
• Molecule 1: Protein S100-A1

Chain A: 43% 46% 6% 5%



• Molecule 1: Protein S100-A1

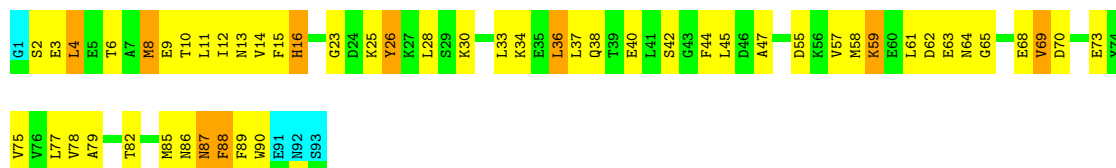
Chain B: 28% 54% 13% 5%



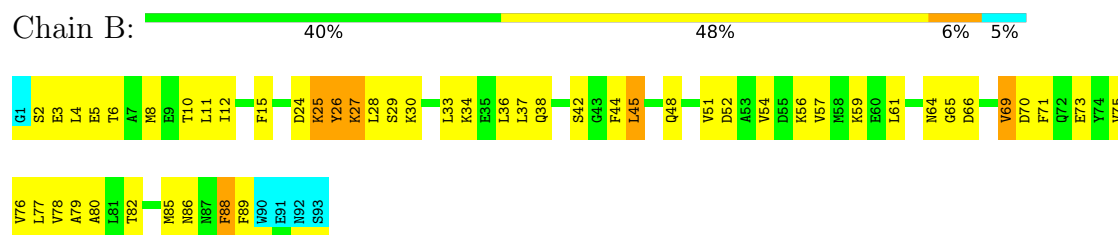
#### 4.2.19 Score per residue for model 19

• Molecule 1: Protein S100-A1

Chain A: 40% 46% 10% 4%

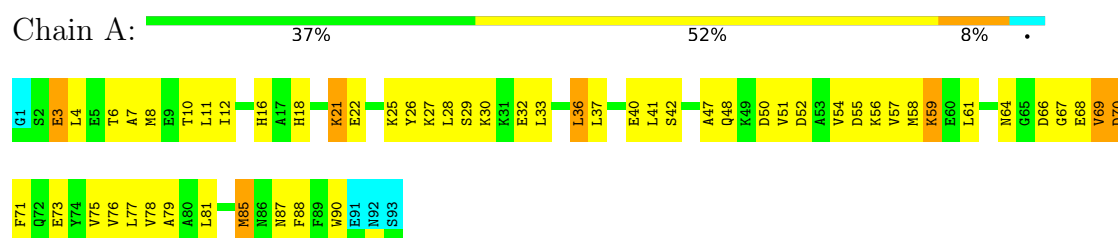


- Molecule 1: Protein S100-A1

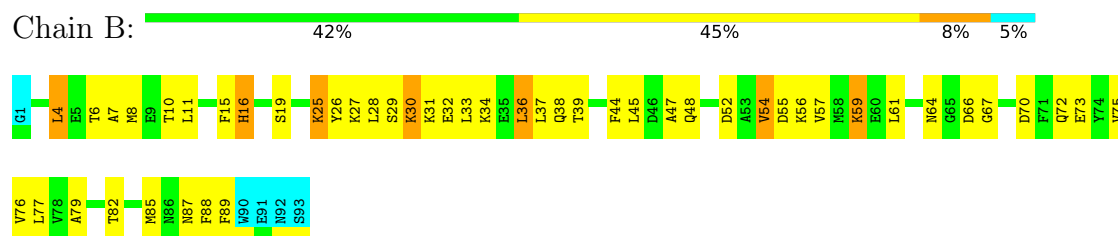


#### 4.2.20 Score per residue for model 20

- Molecule 1: Protein S100-A1



- Molecule 1: Protein S100-A1



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR NIH    | refinement         | 2.26    |
| CYANA         | structure solution |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1148           |
| Number of shifts mapped to atoms             | 1148           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 47%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.86±0.02    | 0±0/717 ( 0.0± 0.0%) | 1.06±0.02   | 1±1/966 ( 0.1± 0.1%) |
| 1   | B     | 0.86±0.02    | 0±0/701 ( 0.0± 0.0%) | 1.05±0.02   | 1±1/943 ( 0.1± 0.1%) |
| All | All   | 0.86         | 0/28360 ( 0.0%)      | 1.05        | 33/38180 ( 0.1%)     |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 1   | A     | 18  | HIS  | CA-CB-CG | -6.50 | 107.30      | 113.80   | 7      | 12    |
| 1   | B     | 16  | HIS  | CA-CB-CG | -5.98 | 107.82      | 113.80   | 11     | 5     |
| 1   | B     | 88  | PHE  | CA-CB-CG | -5.89 | 107.91      | 113.80   | 10     | 4     |
| 1   | B     | 18  | HIS  | CA-CB-CG | -5.70 | 108.11      | 113.80   | 1      | 7     |
| 1   | B     | 71  | PHE  | CA-CB-CG | -5.65 | 108.15      | 113.80   | 3      | 2     |
| 1   | A     | 63  | GLU  | N-CA-C   | -5.34 | 105.46      | 111.28   | 10     | 1     |
| 1   | A     | 65  | GLY  | N-CA-C   | -5.17 | 108.55      | 115.32   | 18     | 1     |
| 1   | A     | 88  | PHE  | CA-CB-CG | -5.05 | 108.75      | 113.80   | 19     | 1     |

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 706   | 690      | 688      | 59±8    |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | B     | 692   | 680      | 678      | 59±10   |
| All | All   | 27960 | 27400    | 27320    | 2055    |

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 37.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:14:VAL:HG21 | 1:B:4:LEU:HD21  | 1.00     | 1.29        | 1      | 4     |
| 1:A:11:LEU:HD23 | 1:B:4:LEU:HD22  | 0.93     | 1.39        | 14     | 9     |
| 1:A:14:VAL:HG21 | 1:B:4:LEU:HD11  | 0.89     | 1.42        | 13     | 9     |
| 1:A:75:VAL:HG21 | 1:B:79:ALA:CB   | 0.89     | 1.96        | 12     | 20    |
| 1:B:47:ALA:HB3  | 1:B:85:MET:SD   | 0.89     | 2.07        | 18     | 8     |
| 1:B:57:VAL:HG12 | 1:B:77:LEU:HD12 | 0.87     | 1.45        | 3      | 15    |
| 1:A:47:ALA:HB3  | 1:A:85:MET:SD   | 0.86     | 2.11        | 10     | 11    |
| 1:A:79:ALA:CB   | 1:B:75:VAL:HG21 | 0.86     | 2.00        | 19     | 20    |
| 1:A:11:LEU:HD11 | 1:B:8:MET:SD    | 0.85     | 2.11        | 9      | 13    |
| 1:A:35:GLU:O    | 1:A:39:THR:HG22 | 0.83     | 1.73        | 15     | 1     |
| 1:A:4:LEU:CD1   | 1:B:11:LEU:HD23 | 0.82     | 2.02        | 10     | 9     |
| 1:A:11:LEU:HD23 | 1:B:4:LEU:HD12  | 0.82     | 1.50        | 8      | 4     |
| 1:A:61:LEU:HG   | 1:A:77:LEU:HD13 | 0.82     | 1.51        | 16     | 12    |
| 1:A:33:LEU:HD11 | 1:A:77:LEU:HD22 | 0.82     | 1.52        | 14     | 6     |
| 1:B:69:VAL:HG23 | 1:B:73:GLU:HB2  | 0.81     | 1.51        | 7      | 7     |
| 1:B:69:VAL:HG23 | 1:B:73:GLU:CB   | 0.80     | 2.06        | 9      | 11    |
| 1:B:33:LEU:HD11 | 1:B:77:LEU:CD2  | 0.80     | 2.06        | 14     | 11    |
| 1:A:51:VAL:O    | 1:A:54:VAL:HG12 | 0.80     | 1.76        | 20     | 10    |
| 1:A:4:LEU:HD13  | 1:B:11:LEU:CD2  | 0.79     | 2.07        | 1      | 5     |
| 1:A:69:VAL:HG23 | 1:A:73:GLU:HB2  | 0.78     | 1.54        | 14     | 13    |
| 1:A:4:LEU:HD23  | 1:B:40:GLU:CB   | 0.78     | 2.09        | 17     | 1     |
| 1:A:33:LEU:HD11 | 1:A:77:LEU:CD2  | 0.77     | 2.10        | 13     | 14    |
| 1:A:4:LEU:HD21  | 1:B:14:VAL:HG21 | 0.76     | 1.54        | 11     | 13    |
| 1:A:53:ALA:O    | 1:A:57:VAL:HG23 | 0.75     | 1.82        | 16     | 13    |
| 1:A:57:VAL:HG12 | 1:A:77:LEU:HD12 | 0.75     | 1.57        | 5      | 16    |
| 1:A:4:LEU:HD21  | 1:B:74:TYR:OH   | 0.74     | 1.81        | 17     | 1     |
| 1:B:37:LEU:HD11 | 1:B:81:LEU:CD1  | 0.74     | 2.12        | 14     | 6     |
| 1:A:4:LEU:HD13  | 1:B:11:LEU:HD23 | 0.74     | 1.58        | 10     | 9     |
| 1:A:12:ILE:HG21 | 1:B:86:ASN:ND2  | 0.74     | 1.96        | 17     | 1     |
| 1:B:33:LEU:HD21 | 1:B:77:LEU:HD23 | 0.74     | 1.57        | 16     | 10    |
| 1:B:36:LEU:HD21 | 1:B:74:TYR:CE1  | 0.74     | 2.17        | 17     | 10    |
| 1:A:37:LEU:HD12 | 1:A:58:MET:SD   | 0.74     | 2.23        | 11     | 2     |
| 1:A:69:VAL:HG23 | 1:A:73:GLU:CB   | 0.73     | 2.13        | 1      | 13    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:12:ILE:HG22 | 1:B:16:HIS:CD2  | 0.73     | 2.19        | 6      | 2     |
| 1:A:40:GLU:HB3  | 1:B:4:LEU:HD12  | 0.72     | 1.60        | 19     | 8     |
| 1:B:82:THR:HG22 | 1:B:86:ASN:OD1  | 0.71     | 1.85        | 16     | 3     |
| 1:B:44:PHE:CE1  | 1:B:85:MET:HE2  | 0.71     | 2.20        | 17     | 5     |
| 1:B:18:HIS:CD2  | 1:B:36:LEU:HD13 | 0.71     | 2.21        | 8      | 2     |
| 1:A:47:ALA:HB1  | 1:A:85:MET:HE2  | 0.71     | 1.61        | 17     | 1     |
| 1:B:51:VAL:O    | 1:B:54:VAL:HG12 | 0.70     | 1.86        | 11     | 8     |
| 1:A:4:LEU:HD23  | 1:B:40:GLU:HB3  | 0.70     | 1.64        | 17     | 1     |
| 1:A:71:PHE:O    | 1:A:75:VAL:HG22 | 0.69     | 1.87        | 1      | 11    |
| 1:A:61:LEU:CD1  | 1:A:77:LEU:HD22 | 0.69     | 2.17        | 5      | 1     |
| 1:B:61:LEU:HG   | 1:B:77:LEU:HD13 | 0.69     | 1.62        | 1      | 12    |
| 1:A:33:LEU:C    | 1:A:33:LEU:HD13 | 0.68     | 2.13        | 16     | 20    |
| 1:B:69:VAL:HG23 | 1:B:73:GLU:HB3  | 0.68     | 1.65        | 3      | 6     |
| 1:B:37:LEU:C    | 1:B:37:LEU:HD13 | 0.68     | 2.14        | 18     | 18    |
| 1:A:37:LEU:HD11 | 1:A:81:LEU:CD1  | 0.68     | 2.18        | 8      | 5     |
| 1:A:4:LEU:HD12  | 1:B:11:LEU:HD23 | 0.68     | 1.63        | 8      | 4     |
| 1:A:47:ALA:CB   | 1:A:85:MET:SD   | 0.67     | 2.82        | 9      | 9     |
| 1:B:33:LEU:C    | 1:B:33:LEU:HD13 | 0.67     | 2.15        | 6      | 20    |
| 1:A:12:ILE:HG21 | 1:B:86:ASN:OD1  | 0.67     | 1.90        | 8      | 1     |
| 1:A:44:PHE:HA   | 1:A:85:MET:SD   | 0.67     | 2.30        | 15     | 5     |
| 1:A:40:GLU:HB3  | 1:B:4:LEU:HD23  | 0.67     | 1.67        | 7      | 1     |
| 1:B:30:LYS:NZ   | 1:B:62:ASP:HA   | 0.67     | 2.05        | 10     | 2     |
| 1:A:37:LEU:C    | 1:A:37:LEU:HD13 | 0.66     | 2.15        | 20     | 19    |
| 1:A:70:ASP:CG   | 1:A:71:PHE:N    | 0.66     | 2.53        | 12     | 8     |
| 1:B:37:LEU:HD21 | 1:B:41:LEU:HD22 | 0.66     | 1.65        | 7      | 4     |
| 1:A:8:MET:SD    | 1:B:11:LEU:HD11 | 0.66     | 2.30        | 3      | 6     |
| 1:B:44:PHE:CE2  | 1:B:85:MET:HE2  | 0.66     | 2.26        | 20     | 1     |
| 1:B:53:ALA:O    | 1:B:57:VAL:HG23 | 0.66     | 1.91        | 16     | 7     |
| 1:A:33:LEU:HD22 | 1:A:33:LEU:O    | 0.66     | 1.90        | 5      | 4     |
| 1:A:90:TRP:CD1  | 1:A:90:TRP:N    | 0.66     | 2.61        | 19     | 11    |
| 1:A:12:ILE:HG21 | 1:B:86:ASN:HD21 | 0.66     | 1.49        | 17     | 1     |
| 1:A:75:VAL:HG21 | 1:B:79:ALA:HB1  | 0.65     | 1.68        | 5      | 7     |
| 1:A:33:LEU:HD21 | 1:A:77:LEU:HD23 | 0.65     | 1.69        | 7      | 12    |
| 1:B:79:ALA:O    | 1:B:83:VAL:HG12 | 0.65     | 1.90        | 3      | 1     |
| 1:B:70:ASP:CG   | 1:B:71:PHE:N    | 0.65     | 2.55        | 16     | 9     |
| 1:A:28:LEU:HD21 | 1:A:33:LEU:HD23 | 0.65     | 1.69        | 6      | 4     |
| 1:A:30:LYS:NZ   | 1:A:62:ASP:HA   | 0.65     | 2.07        | 15     | 2     |
| 1:A:33:LEU:HD21 | 1:A:77:LEU:CD2  | 0.64     | 2.22        | 16     | 7     |
| 1:B:85:MET:HE1  | 1:B:89:PHE:CE2  | 0.64     | 2.27        | 15     | 2     |
| 1:A:33:LEU:HB2  | 1:A:69:VAL:HG11 | 0.63     | 1.68        | 2      | 5     |
| 1:B:37:LEU:HD11 | 1:B:81:LEU:HD11 | 0.63     | 1.70        | 10     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:44:PHE:CE2  | 1:A:85:MET:HE2  | 0.63     | 2.28        | 15     | 2     |
| 1:A:61:LEU:HG   | 1:A:77:LEU:HD22 | 0.63     | 1.70        | 9      | 7     |
| 1:B:37:LEU:HD21 | 1:B:81:LEU:HD12 | 0.63     | 1.70        | 16     | 3     |
| 1:B:30:LYS:NZ   | 1:B:61:LEU:O    | 0.62     | 2.33        | 4      | 5     |
| 1:A:86:ASN:CG   | 1:B:12:ILE:HG21 | 0.62     | 2.19        | 6      | 4     |
| 1:A:69:VAL:HG23 | 1:A:73:GLU:HB3  | 0.62     | 1.72        | 1      | 1     |
| 1:B:37:LEU:HD23 | 1:B:78:VAL:HG12 | 0.62     | 1.72        | 14     | 12    |
| 1:A:37:LEU:HD21 | 1:A:81:LEU:HD12 | 0.62     | 1.71        | 1      | 2     |
| 1:A:47:ALA:HB1  | 1:A:85:MET:CE   | 0.62     | 2.25        | 17     | 1     |
| 1:A:16:HIS:NE2  | 1:B:86:ASN:OD1  | 0.61     | 2.31        | 11     | 4     |
| 1:B:16:HIS:CE1  | 1:B:26:TYR:HB3  | 0.61     | 2.30        | 2      | 6     |
| 1:B:47:ALA:CB   | 1:B:85:MET:SD   | 0.61     | 2.88        | 17     | 7     |
| 1:A:16:HIS:ND1  | 1:A:25:LYS:O    | 0.61     | 2.33        | 13     | 2     |
| 1:A:78:VAL:HG23 | 1:B:8:MET:SD    | 0.61     | 2.36        | 17     | 2     |
| 1:A:36:LEU:HD21 | 1:A:74:TYR:CE1  | 0.61     | 2.31        | 10     | 6     |
| 1:B:12:ILE:HD13 | 1:B:71:PHE:CD1  | 0.61     | 2.30        | 3      | 9     |
| 1:B:59:LYS:HB2  | 1:B:59:LYS:NZ   | 0.61     | 2.11        | 8      | 1     |
| 1:B:35:GLU:O    | 1:B:39:THR:HG22 | 0.61     | 1.96        | 14     | 1     |
| 1:B:71:PHE:O    | 1:B:75:VAL:HG22 | 0.60     | 1.96        | 19     | 9     |
| 1:A:90:TRP:CD1  | 1:A:90:TRP:H    | 0.60     | 2.14        | 12     | 4     |
| 1:B:33:LEU:HD21 | 1:B:77:LEU:CD2  | 0.60     | 2.27        | 9      | 2     |
| 1:B:45:LEU:HD12 | 1:B:45:LEU:O    | 0.60     | 1.95        | 18     | 12    |
| 1:A:56:LYS:CD   | 1:A:56:LYS:N    | 0.60     | 2.64        | 9      | 2     |
| 1:B:36:LEU:HD12 | 1:B:36:LEU:C    | 0.60     | 2.22        | 15     | 9     |
| 1:A:86:ASN:OD1  | 1:A:90:TRP:NE1  | 0.60     | 2.33        | 10     | 7     |
| 1:B:44:PHE:CD1  | 1:B:85:MET:SD   | 0.60     | 2.95        | 12     | 4     |
| 1:A:10:THR:HG22 | 1:B:4:LEU:CD1   | 0.60     | 2.27        | 9      | 2     |
| 1:A:37:LEU:HD21 | 1:A:41:LEU:HD22 | 0.60     | 1.72        | 7      | 7     |
| 1:B:38:GLN:HB2  | 1:B:45:LEU:HD22 | 0.59     | 1.73        | 7      | 4     |
| 1:B:36:LEU:HD12 | 1:B:40:GLU:HG2  | 0.59     | 1.73        | 8      | 2     |
| 1:B:56:LYS:N    | 1:B:56:LYS:CD   | 0.59     | 2.65        | 17     | 1     |
| 1:B:25:LYS:NZ   | 1:B:26:TYR:OH   | 0.59     | 2.31        | 17     | 6     |
| 1:A:90:TRP:CE3  | 1:B:16:HIS:CE1  | 0.59     | 2.90        | 18     | 1     |
| 1:A:55:ASP:O    | 1:A:59:LYS:N    | 0.59     | 2.35        | 10     | 10    |
| 1:A:7:ALA:HB1   | 1:B:7:ALA:HB1   | 0.59     | 1.75        | 20     | 3     |
| 1:B:37:LEU:CD2  | 1:B:41:LEU:HD22 | 0.59     | 2.27        | 7      | 1     |
| 1:B:85:MET:O    | 1:B:85:MET:HE2  | 0.59     | 1.98        | 9      | 1     |
| 1:B:18:HIS:CD2  | 1:B:36:LEU:HD22 | 0.59     | 2.33        | 4      | 4     |
| 1:A:54:VAL:HA   | 1:A:81:LEU:HD21 | 0.59     | 1.75        | 5      | 2     |
| 1:B:46:ASP:O    | 1:B:49:LYS:NZ   | 0.59     | 2.36        | 13     | 3     |
| 1:A:14:VAL:HG21 | 1:B:4:LEU:CD2   | 0.59     | 2.19        | 1      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:86:ASN:O    | 1:A:90:TRP:CD1  | 0.59     | 2.56        | 12     | 6     |
| 1:B:57:VAL:HG11 | 1:B:81:LEU:HG   | 0.59     | 1.74        | 16     | 3     |
| 1:B:44:PHE:CE2  | 1:B:82:THR:HG23 | 0.59     | 2.33        | 14     | 2     |
| 1:A:37:LEU:HD23 | 1:A:78:VAL:HG12 | 0.58     | 1.73        | 7      | 15    |
| 1:A:48:GLN:HE22 | 1:A:54:VAL:HG21 | 0.58     | 1.58        | 7      | 1     |
| 1:A:58:MET:O    | 1:A:62:ASP:N    | 0.58     | 2.36        | 2      | 4     |
| 1:A:46:ASP:O    | 1:A:49:LYS:NZ   | 0.58     | 2.36        | 7      | 2     |
| 1:A:85:MET:HE1  | 1:A:89:PHE:CE2  | 0.58     | 2.33        | 8      | 1     |
| 1:A:87:ASN:HA   | 1:A:90:TRP:CD2  | 0.58     | 2.32        | 10     | 2     |
| 1:A:36:LEU:C    | 1:A:36:LEU:HD12 | 0.58     | 2.24        | 17     | 6     |
| 1:B:61:LEU:O    | 1:B:65:GLY:N    | 0.58     | 2.35        | 9      | 5     |
| 1:A:30:LYS:NZ   | 1:A:62:ASP:O    | 0.58     | 2.36        | 4      | 3     |
| 1:A:86:ASN:O    | 1:A:89:PHE:N    | 0.58     | 2.37        | 12     | 4     |
| 1:B:52:ASP:OD2  | 1:B:56:LYS:NZ   | 0.58     | 2.37        | 9      | 8     |
| 1:A:30:LYS:NZ   | 1:A:65:GLY:O    | 0.58     | 2.37        | 8      | 3     |
| 1:A:14:VAL:CG2  | 1:B:4:LEU:HD11  | 0.57     | 2.24        | 13     | 2     |
| 1:B:61:LEU:HG   | 1:B:77:LEU:HD22 | 0.57     | 1.75        | 12     | 6     |
| 1:A:30:LYS:NZ   | 1:A:68:GLU:O    | 0.57     | 2.38        | 20     | 3     |
| 1:B:55:ASP:O    | 1:B:59:LYS:N    | 0.57     | 2.36        | 2      | 11    |
| 1:B:37:LEU:HD12 | 1:B:77:LEU:HD21 | 0.57     | 1.75        | 10     | 1     |
| 1:B:8:MET:SD    | 1:B:11:LEU:HD12 | 0.57     | 2.40        | 1      | 4     |
| 1:A:28:LEU:HD11 | 1:A:32:GLU:HB2  | 0.57     | 1.77        | 13     | 3     |
| 1:A:17:ALA:O    | 1:A:21:LYS:NZ   | 0.57     | 2.38        | 3      | 3     |
| 1:A:30:LYS:NZ   | 1:A:64:ASN:OD1  | 0.57     | 2.38        | 3      | 1     |
| 1:B:30:LYS:NZ   | 1:B:68:GLU:O    | 0.57     | 2.38        | 17     | 1     |
| 1:A:79:ALA:O    | 1:A:83:VAL:HG12 | 0.56     | 2.00        | 3      | 4     |
| 1:B:51:VAL:HG12 | 1:B:51:VAL:O    | 0.56     | 2.00        | 14     | 1     |
| 1:A:86:ASN:OD1  | 1:B:12:ILE:HG21 | 0.56     | 2.00        | 19     | 4     |
| 1:A:34:LYS:HZ2  | 1:A:34:LYS:HB2  | 0.56     | 1.60        | 4      | 1     |
| 1:B:30:LYS:NZ   | 1:B:64:ASN:OD1  | 0.56     | 2.35        | 7      | 2     |
| 1:A:44:PHE:CD1  | 1:A:85:MET:SD   | 0.56     | 2.99        | 11     | 5     |
| 1:B:48:GLN:HE22 | 1:B:54:VAL:HG21 | 0.56     | 1.61        | 13     | 1     |
| 1:A:70:ASP:CG   | 1:A:71:PHE:H    | 0.56     | 2.08        | 10     | 6     |
| 1:B:24:ASP:CG   | 1:B:25:LYS:H    | 0.56     | 2.08        | 2      | 4     |
| 1:B:87:ASN:C    | 1:B:87:ASN:HD22 | 0.56     | 2.07        | 9      | 2     |
| 1:A:14:VAL:HG11 | 1:B:4:LEU:HD11  | 0.56     | 1.76        | 4      | 1     |
| 1:A:34:LYS:CB   | 1:A:34:LYS:NZ   | 0.56     | 2.68        | 4      | 1     |
| 1:B:30:LYS:NZ   | 1:B:64:ASN:O    | 0.56     | 2.38        | 14     | 4     |
| 1:B:45:LEU:HD12 | 1:B:48:GLN:NE2  | 0.56     | 2.15        | 14     | 1     |
| 1:A:4:LEU:HD11  | 1:B:74:TYR:OH   | 0.56     | 2.01        | 14     | 3     |
| 1:B:28:LEU:O    | 1:B:69:VAL:HG13 | 0.56     | 2.01        | 9      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:30:LYS:NZ   | 1:A:64:ASN:O    | 0.56     | 2.36        | 13     | 8     |
| 1:B:53:ALA:O    | 1:B:57:VAL:N    | 0.56     | 2.34        | 9      | 2     |
| 1:B:61:LEU:HD13 | 1:B:64:ASN:OD1  | 0.56     | 2.00        | 20     | 1     |
| 1:A:28:LEU:HD11 | 1:A:32:GLU:CB   | 0.55     | 2.31        | 2      | 2     |
| 1:B:64:ASN:C    | 1:B:66:ASP:H    | 0.55     | 2.10        | 5      | 11    |
| 1:B:4:LEU:N     | 1:B:4:LEU:CD2   | 0.55     | 2.69        | 8      | 1     |
| 1:A:28:LEU:CD2  | 1:A:33:LEU:HD23 | 0.55     | 2.30        | 6      | 3     |
| 1:A:83:VAL:HG11 | 1:B:72:GLN:HG3  | 0.55     | 1.78        | 7      | 4     |
| 1:A:27:LYS:NZ   | 1:A:70:ASP:HB2  | 0.55     | 2.16        | 12     | 1     |
| 1:A:87:ASN:HD22 | 1:A:87:ASN:C    | 0.55     | 2.09        | 19     | 2     |
| 1:B:30:LYS:O    | 1:B:34:LYS:NZ   | 0.55     | 2.38        | 6      | 7     |
| 1:B:80:ALA:O    | 1:B:83:VAL:HG12 | 0.55     | 2.02        | 11     | 5     |
| 1:A:37:LEU:CD2  | 1:A:41:LEU:HD22 | 0.55     | 2.31        | 3      | 4     |
| 1:B:37:LEU:HD22 | 1:B:37:LEU:O    | 0.55     | 2.01        | 3      | 3     |
| 1:B:37:LEU:HD12 | 1:B:58:MET:SD   | 0.55     | 2.41        | 11     | 3     |
| 1:A:57:VAL:HG11 | 1:A:81:LEU:HG   | 0.55     | 1.79        | 14     | 2     |
| 1:A:25:LYS:HG3  | 1:A:26:TYR:CE2  | 0.55     | 2.37        | 5      | 1     |
| 1:B:22:GLU:O    | 1:B:24:ASP:N    | 0.55     | 2.40        | 8      | 2     |
| 1:A:78:VAL:CG2  | 1:B:8:MET:SD    | 0.55     | 2.95        | 17     | 1     |
| 1:A:64:ASN:C    | 1:A:66:ASP:H    | 0.55     | 2.10        | 7      | 6     |
| 1:B:30:LYS:N    | 1:B:67:GLY:O    | 0.55     | 2.38        | 17     | 1     |
| 1:B:58:MET:O    | 1:B:62:ASP:N    | 0.54     | 2.40        | 16     | 3     |
| 1:B:25:LYS:NZ   | 1:B:26:TYR:CZ   | 0.54     | 2.75        | 13     | 2     |
| 1:A:68:GLU:N    | 1:A:68:GLU:CD   | 0.54     | 2.64        | 1      | 2     |
| 1:A:85:MET:O    | 1:A:89:PHE:N    | 0.54     | 2.37        | 2      | 1     |
| 1:B:33:LEU:HD11 | 1:B:77:LEU:HD21 | 0.54     | 1.77        | 8      | 2     |
| 1:A:4:LEU:CD2   | 1:B:14:VAL:HG21 | 0.54     | 2.31        | 4      | 5     |
| 1:A:12:ILE:HD13 | 1:A:71:PHE:CD1  | 0.54     | 2.37        | 17     | 10    |
| 1:A:51:VAL:O    | 1:A:53:ALA:N    | 0.54     | 2.36        | 10     | 6     |
| 1:A:22:GLU:CD   | 1:A:29:SER:H    | 0.54     | 2.10        | 16     | 4     |
| 1:A:30:LYS:N    | 1:A:30:LYS:HD2  | 0.54     | 2.18        | 14     | 1     |
| 1:A:90:TRP:NE1  | 1:B:16:HIS:CE1  | 0.54     | 2.75        | 2      | 2     |
| 1:B:33:LEU:HD11 | 1:B:77:LEU:HD22 | 0.54     | 1.80        | 3      | 4     |
| 1:B:15:PHE:CE1  | 1:B:28:LEU:HB2  | 0.54     | 2.37        | 12     | 5     |
| 1:B:44:PHE:CZ   | 1:B:82:THR:HG23 | 0.54     | 2.38        | 17     | 4     |
| 1:B:70:ASP:CG   | 1:B:71:PHE:H    | 0.54     | 2.11        | 4      | 6     |
| 1:A:57:VAL:CG1  | 1:A:77:LEU:HD12 | 0.54     | 2.33        | 16     | 6     |
| 1:A:52:ASP:CG   | 1:A:56:LYS:HZ3  | 0.54     | 2.10        | 1      | 1     |
| 1:A:38:GLN:HA   | 1:A:45:LEU:HD22 | 0.54     | 1.80        | 6      | 5     |
| 1:B:3:GLU:CD    | 1:B:3:GLU:H     | 0.54     | 2.10        | 18     | 3     |
| 1:B:16:HIS:CE1  | 1:B:26:TYR:CB   | 0.54     | 2.91        | 20     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:16:HIS:ND1  | 1:B:25:LYS:O    | 0.54     | 2.40        | 16     | 3     |
| 1:A:14:VAL:HG11 | 1:A:40:GLU:HG2  | 0.54     | 1.79        | 8      | 1     |
| 1:A:59:LYS:HB2  | 1:A:59:LYS:NZ   | 0.54     | 2.18        | 20     | 1     |
| 1:B:33:LEU:HD22 | 1:B:33:LEU:O    | 0.54     | 2.03        | 9      | 7     |
| 1:A:86:ASN:ND2  | 1:B:12:ILE:HG13 | 0.54     | 2.18        | 12     | 2     |
| 1:B:86:ASN:O    | 1:B:89:PHE:N    | 0.53     | 2.41        | 7      | 4     |
| 1:B:30:LYS:HG3  | 1:B:65:GLY:CA   | 0.53     | 2.32        | 17     | 1     |
| 1:B:4:LEU:N     | 1:B:4:LEU:HD22  | 0.53     | 2.19        | 8      | 1     |
| 1:B:48:GLN:NE2  | 1:B:85:MET:SD   | 0.53     | 2.82        | 11     | 1     |
| 1:B:32:GLU:O    | 1:B:36:LEU:N    | 0.53     | 2.31        | 7      | 5     |
| 1:B:36:LEU:HD12 | 1:B:40:GLU:CG   | 0.53     | 2.33        | 8      | 2     |
| 1:B:30:LYS:NZ   | 1:B:62:ASP:O    | 0.53     | 2.38        | 15     | 3     |
| 1:A:45:LEU:HD12 | 1:A:48:GLN:NE2  | 0.53     | 2.19        | 16     | 1     |
| 1:B:44:PHE:HA   | 1:B:85:MET:SD   | 0.53     | 2.43        | 16     | 6     |
| 1:B:46:ASP:OD1  | 1:B:49:LYS:NZ   | 0.53     | 2.41        | 2      | 5     |
| 1:A:64:ASN:C    | 1:A:66:ASP:N    | 0.53     | 2.67        | 7      | 2     |
| 1:A:90:TRP:HZ2  | 1:B:12:ILE:HD12 | 0.53     | 1.62        | 9      | 3     |
| 1:A:61:LEU:O    | 1:A:65:GLY:N    | 0.53     | 2.42        | 2      | 3     |
| 1:A:75:VAL:HG21 | 1:B:79:ALA:HB2  | 0.53     | 1.78        | 13     | 5     |
| 1:A:64:ASN:O    | 1:A:66:ASP:N    | 0.53     | 2.38        | 6      | 4     |
| 1:B:64:ASN:O    | 1:B:66:ASP:N    | 0.53     | 2.39        | 15     | 4     |
| 1:B:52:ASP:OD1  | 1:B:56:LYS:NZ   | 0.53     | 2.39        | 5      | 2     |
| 1:B:22:GLU:HG3  | 1:B:32:GLU:CG   | 0.53     | 2.33        | 7      | 1     |
| 1:A:18:HIS:CE1  | 1:A:36:LEU:HB2  | 0.53     | 2.39        | 20     | 1     |
| 1:A:47:ALA:HB1  | 1:A:85:MET:HE3  | 0.53     | 1.81        | 1      | 3     |
| 1:B:48:GLN:CG   | 1:B:85:MET:SD   | 0.53     | 2.98        | 8      | 1     |
| 1:A:28:LEU:O    | 1:A:69:VAL:N    | 0.52     | 2.28        | 2      | 5     |
| 1:A:59:LYS:O    | 1:A:63:GLU:N    | 0.52     | 2.38        | 7      | 5     |
| 1:A:22:GLU:OE1  | 1:A:29:SER:N    | 0.52     | 2.41        | 5      | 6     |
| 1:A:79:ALA:HB3  | 1:B:75:VAL:HG21 | 0.52     | 1.79        | 19     | 4     |
| 1:B:27:LYS:NZ   | 1:B:70:ASP:HB3  | 0.52     | 2.18        | 14     | 1     |
| 1:B:22:GLU:OE1  | 1:B:29:SER:N    | 0.52     | 2.43        | 18     | 7     |
| 1:A:30:LYS:NZ   | 1:A:61:LEU:O    | 0.52     | 2.38        | 17     | 5     |
| 1:B:31:LYS:O    | 1:B:34:LYS:NZ   | 0.52     | 2.42        | 20     | 1     |
| 1:B:24:ASP:CG   | 1:B:25:LYS:N    | 0.52     | 2.67        | 14     | 4     |
| 1:B:51:VAL:O    | 1:B:53:ALA:N    | 0.52     | 2.43        | 13     | 5     |
| 1:B:64:ASN:HD22 | 1:B:73:GLU:CD   | 0.52     | 2.12        | 3      | 1     |
| 1:A:61:LEU:HD11 | 1:A:73:GLU:O    | 0.52     | 2.05        | 12     | 2     |
| 1:B:48:GLN:HE22 | 1:B:51:VAL:HG11 | 0.52     | 1.64        | 4      | 1     |
| 1:A:8:MET:SD    | 1:B:78:VAL:HG23 | 0.52     | 2.44        | 4      | 1     |
| 1:B:15:PHE:CE2  | 1:B:28:LEU:HB2  | 0.52     | 2.39        | 11     | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:76:VAL:O    | 1:A:80:ALA:N    | 0.52     | 2.36        | 12     | 5     |
| 1:B:28:LEU:O    | 1:B:69:VAL:N    | 0.52     | 2.38        | 17     | 3     |
| 1:B:30:LYS:NZ   | 1:B:65:GLY:O    | 0.52     | 2.37        | 8      | 4     |
| 1:A:8:MET:SD    | 1:B:82:THR:OG1  | 0.52     | 2.68        | 19     | 1     |
| 1:A:52:ASP:OD2  | 1:A:56:LYS:NZ   | 0.52     | 2.42        | 12     | 7     |
| 1:A:51:VAL:O    | 1:A:51:VAL:HG12 | 0.52     | 2.04        | 10     | 1     |
| 1:A:85:MET:HE3  | 1:A:89:PHE:CZ   | 0.52     | 2.40        | 10     | 1     |
| 1:B:45:LEU:HA   | 1:B:48:GLN:NE2  | 0.52     | 2.20        | 10     | 1     |
| 1:B:44:PHE:CD1  | 1:B:85:MET:HE2  | 0.51     | 2.40        | 3      | 3     |
| 1:B:85:MET:HE3  | 1:B:89:PHE:CE1  | 0.51     | 2.39        | 1      | 1     |
| 1:A:8:MET:HE2   | 1:B:78:VAL:HG23 | 0.51     | 1.82        | 8      | 5     |
| 1:B:48:GLN:HG2  | 1:B:85:MET:SD   | 0.51     | 2.44        | 8      | 2     |
| 1:B:30:LYS:HZ1  | 1:B:62:ASP:HA   | 0.51     | 1.64        | 10     | 2     |
| 1:A:11:LEU:CD2  | 1:B:4:LEU:HD12  | 0.51     | 2.36        | 10     | 1     |
| 1:A:11:LEU:CD2  | 1:B:4:LEU:HD22  | 0.51     | 2.28        | 14     | 3     |
| 1:B:51:VAL:C    | 1:B:53:ALA:H    | 0.51     | 2.12        | 9      | 4     |
| 1:B:37:LEU:C    | 1:B:37:LEU:CD2  | 0.51     | 2.84        | 10     | 1     |
| 1:B:59:LYS:O    | 1:B:63:GLU:N    | 0.51     | 2.41        | 3      | 4     |
| 1:A:55:ASP:OD1  | 1:A:59:LYS:NZ   | 0.51     | 2.44        | 19     | 2     |
| 1:B:30:LYS:HG3  | 1:B:65:GLY:HA2  | 0.51     | 1.80        | 17     | 1     |
| 1:A:28:LEU:HB3  | 1:A:69:VAL:O    | 0.51     | 2.06        | 1      | 2     |
| 1:A:70:ASP:O    | 1:A:74:TYR:N    | 0.51     | 2.35        | 1      | 3     |
| 1:B:41:LEU:O    | 1:B:45:LEU:N    | 0.51     | 2.38        | 7      | 1     |
| 1:A:83:VAL:HG23 | 1:A:90:TRP:CZ3  | 0.51     | 2.41        | 9      | 1     |
| 1:A:90:TRP:CE2  | 1:B:16:HIS:CD2  | 0.51     | 2.98        | 11     | 1     |
| 1:A:27:LYS:NZ   | 1:A:70:ASP:CB   | 0.51     | 2.73        | 12     | 1     |
| 1:A:14:VAL:HG21 | 1:B:4:LEU:HD23  | 0.51     | 1.80        | 17     | 1     |
| 1:A:45:LEU:HD13 | 1:A:58:MET:HE1  | 0.51     | 1.82        | 17     | 1     |
| 1:A:30:LYS:NZ   | 1:A:73:GLU:OE2  | 0.51     | 2.43        | 18     | 1     |
| 1:B:63:GLU:C    | 1:B:65:GLY:H    | 0.51     | 2.14        | 2      | 2     |
| 1:A:59:LYS:NZ   | 1:A:63:GLU:OE2  | 0.51     | 2.43        | 11     | 7     |
| 1:B:30:LYS:CE   | 1:B:62:ASP:HA   | 0.51     | 2.36        | 11     | 1     |
| 1:A:30:LYS:HZ3  | 1:A:64:ASN:C    | 0.51     | 2.13        | 3      | 1     |
| 1:A:44:PHE:CZ   | 1:A:82:THR:HG23 | 0.51     | 2.40        | 16     | 4     |
| 1:A:44:PHE:CD1  | 1:A:85:MET:HE2  | 0.51     | 2.40        | 10     | 2     |
| 1:A:33:LEU:HD22 | 1:A:33:LEU:C    | 0.51     | 2.31        | 5      | 1     |
| 1:B:55:ASP:OD1  | 1:B:59:LYS:NZ   | 0.51     | 2.44        | 17     | 6     |
| 1:A:34:LYS:NZ   | 1:A:62:ASP:OD2  | 0.51     | 2.40        | 10     | 2     |
| 1:B:25:LYS:HG2  | 1:B:26:TYR:N    | 0.51     | 2.21        | 4      | 1     |
| 1:A:86:ASN:HB3  | 1:A:90:TRP:CZ2  | 0.51     | 2.41        | 8      | 2     |
| 1:B:55:ASP:OD2  | 1:B:59:LYS:NZ   | 0.51     | 2.44        | 12     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:15:PHE:CE2  | 1:B:28:LEU:CB   | 0.51     | 2.94        | 20     | 2     |
| 1:B:59:LYS:NZ   | 1:B:63:GLU:OE2  | 0.50     | 2.39        | 6      | 2     |
| 1:B:3:GLU:O     | 1:B:7:ALA:N     | 0.50     | 2.40        | 5      | 4     |
| 1:A:57:VAL:HG12 | 1:A:77:LEU:CD1  | 0.50     | 2.35        | 16     | 9     |
| 1:B:71:PHE:O    | 1:B:75:VAL:HG13 | 0.50     | 2.06        | 17     | 2     |
| 1:A:32:GLU:O    | 1:A:36:LEU:N    | 0.50     | 2.38        | 8      | 6     |
| 1:A:8:MET:HB3   | 1:B:82:THR:HG21 | 0.50     | 1.82        | 8      | 2     |
| 1:A:85:MET:O    | 1:A:85:MET:HE2  | 0.50     | 2.06        | 8      | 2     |
| 1:A:46:ASP:OD1  | 1:A:49:LYS:NZ   | 0.50     | 2.43        | 5      | 5     |
| 1:B:44:PHE:HD1  | 1:B:85:MET:SD   | 0.50     | 2.29        | 10     | 2     |
| 1:B:28:LEU:CD2  | 1:B:33:LEU:HD23 | 0.50     | 2.36        | 12     | 3     |
| 1:A:79:ALA:HB1  | 1:B:75:VAL:HG21 | 0.50     | 1.84        | 5      | 3     |
| 1:B:48:GLN:HG3  | 1:B:85:MET:SD   | 0.50     | 2.46        | 10     | 1     |
| 1:A:48:GLN:CD   | 1:A:54:VAL:HG11 | 0.50     | 2.32        | 17     | 1     |
| 1:B:64:ASN:HD21 | 1:B:73:GLU:CD   | 0.50     | 2.14        | 2      | 2     |
| 1:B:10:THR:O    | 1:B:14:VAL:HG23 | 0.50     | 2.07        | 11     | 4     |
| 1:B:45:LEU:HD12 | 1:B:45:LEU:C    | 0.50     | 2.32        | 13     | 5     |
| 1:B:73:GLU:O    | 1:B:76:VAL:HG22 | 0.50     | 2.06        | 20     | 2     |
| 1:A:30:LYS:O    | 1:A:34:LYS:NZ   | 0.50     | 2.37        | 16     | 2     |
| 1:B:22:GLU:CD   | 1:B:29:SER:H    | 0.50     | 2.14        | 1      | 4     |
| 1:B:38:GLN:HB2  | 1:B:45:LEU:CD2  | 0.50     | 2.36        | 8      | 2     |
| 1:A:27:LYS:NZ   | 1:A:68:GLU:OE1  | 0.50     | 2.43        | 20     | 4     |
| 1:A:34:LYS:NZ   | 1:A:62:ASP:OD1  | 0.50     | 2.44        | 14     | 2     |
| 1:A:78:VAL:HB   | 1:B:8:MET:SD    | 0.49     | 2.47        | 17     | 2     |
| 1:A:23:GLY:O    | 1:A:25:LYS:N    | 0.49     | 2.44        | 6      | 1     |
| 1:A:87:ASN:HA   | 1:A:90:TRP:CD1  | 0.49     | 2.42        | 12     | 1     |
| 1:B:34:LYS:HB2  | 1:B:34:LYS:NZ   | 0.49     | 2.22        | 9      | 1     |
| 1:B:45:LEU:HD12 | 1:B:48:GLN:HE21 | 0.49     | 1.67        | 14     | 1     |
| 1:B:44:PHE:O    | 1:B:48:GLN:N    | 0.49     | 2.45        | 19     | 2     |
| 1:A:15:PHE:CE1  | 1:A:28:LEU:HB2  | 0.49     | 2.43        | 14     | 3     |
| 1:B:27:LYS:NZ   | 1:B:68:GLU:OE2  | 0.49     | 2.44        | 11     | 2     |
| 1:A:30:LYS:HD2  | 1:A:69:VAL:HG12 | 0.49     | 1.83        | 14     | 1     |
| 1:A:57:VAL:HG22 | 1:A:80:ALA:HB1  | 0.49     | 1.84        | 16     | 1     |
| 1:B:16:HIS:CE1  | 1:B:26:TYR:HB2  | 0.49     | 2.42        | 20     | 1     |
| 1:A:90:TRP:CD1  | 1:B:16:HIS:HE2  | 0.49     | 2.26        | 9      | 1     |
| 1:A:90:TRP:CD2  | 1:B:16:HIS:NE2  | 0.49     | 2.80        | 11     | 1     |
| 1:B:85:MET:HE3  | 1:B:89:PHE:CZ   | 0.49     | 2.43        | 18     | 1     |
| 1:B:46:ASP:HA   | 1:B:49:LYS:NZ   | 0.49     | 2.23        | 2      | 1     |
| 1:A:48:GLN:HG3  | 1:A:81:LEU:HD22 | 0.49     | 1.84        | 6      | 1     |
| 1:A:61:LEU:CD2  | 1:A:77:LEU:HD13 | 0.49     | 2.37        | 7      | 1     |
| 1:A:54:VAL:O    | 1:A:58:MET:HG3  | 0.49     | 2.08        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:47:ALA:CB   | 1:B:85:MET:HE2  | 0.49     | 2.38        | 2      | 1     |
| 1:A:30:LYS:NZ   | 1:A:64:ASN:C    | 0.49     | 2.70        | 3      | 1     |
| 1:A:30:LYS:O    | 1:A:34:LYS:CD   | 0.49     | 2.61        | 4      | 1     |
| 1:A:35:GLU:O    | 1:A:39:THR:OG1  | 0.49     | 2.30        | 4      | 7     |
| 1:A:33:LEU:HD11 | 1:A:77:LEU:HD21 | 0.49     | 1.84        | 1      | 1     |
| 1:A:28:LEU:O    | 1:A:69:VAL:HG12 | 0.49     | 2.08        | 6      | 1     |
| 1:A:14:VAL:HG21 | 1:B:4:LEU:CG    | 0.49     | 2.37        | 8      | 1     |
| 1:B:57:VAL:HG11 | 1:B:80:ALA:HB3  | 0.49     | 1.84        | 12     | 1     |
| 1:B:37:LEU:C    | 1:B:37:LEU:CD1  | 0.49     | 2.86        | 18     | 4     |
| 1:B:19:SER:HB3  | 1:B:25:LYS:O    | 0.49     | 2.08        | 20     | 1     |
| 1:B:57:VAL:HG12 | 1:B:77:LEU:CD1  | 0.49     | 2.38        | 10     | 13    |
| 1:A:12:ILE:HG22 | 1:A:16:HIS:CD2  | 0.49     | 2.43        | 5      | 2     |
| 1:A:24:ASP:CG   | 1:A:25:LYS:H    | 0.49     | 2.15        | 12     | 2     |
| 1:B:12:ILE:CG2  | 1:B:16:HIS:CD2  | 0.49     | 2.95        | 6      | 2     |
| 1:B:36:LEU:HD12 | 1:B:36:LEU:O    | 0.49     | 2.07        | 5      | 5     |
| 1:B:56:LYS:O    | 1:B:60:GLU:N    | 0.49     | 2.44        | 9      | 2     |
| 1:B:33:LEU:C    | 1:B:33:LEU:CD1  | 0.48     | 2.86        | 6      | 8     |
| 1:A:2:SER:C     | 1:A:4:LEU:N     | 0.48     | 2.70        | 18     | 6     |
| 1:A:4:LEU:CD2   | 1:A:4:LEU:N     | 0.48     | 2.76        | 13     | 3     |
| 1:A:12:ILE:O    | 1:A:16:HIS:N    | 0.48     | 2.33        | 17     | 4     |
| 1:B:34:LYS:NZ   | 1:B:62:ASP:OD1  | 0.48     | 2.43        | 12     | 2     |
| 1:A:79:ALA:HB2  | 1:B:8:MET:HE1   | 0.48     | 1.84        | 19     | 1     |
| 1:A:90:TRP:CE3  | 1:B:26:TYR:CG   | 0.48     | 3.01        | 10     | 2     |
| 1:A:90:TRP:CH2  | 1:B:12:ILE:HG23 | 0.48     | 2.42        | 7      | 1     |
| 1:A:37:LEU:CD1  | 1:A:58:MET:SD   | 0.48     | 2.99        | 11     | 1     |
| 1:B:57:VAL:HG13 | 1:B:80:ALA:HB3  | 0.48     | 1.85        | 16     | 1     |
| 1:A:15:PHE:CE2  | 1:A:28:LEU:HB2  | 0.48     | 2.44        | 12     | 3     |
| 1:A:18:HIS:CD2  | 1:A:36:LEU:HD13 | 0.48     | 2.43        | 1      | 4     |
| 1:A:14:VAL:CG1  | 1:A:36:LEU:HD13 | 0.48     | 2.39        | 7      | 1     |
| 1:A:45:LEU:O    | 1:A:49:LYS:HG3  | 0.48     | 2.09        | 5      | 4     |
| 1:A:90:TRP:HB3  | 1:B:26:TYR:CD1  | 0.48     | 2.43        | 14     | 1     |
| 1:A:25:LYS:C    | 1:A:26:TYR:CD2  | 0.48     | 2.91        | 4      | 1     |
| 1:B:16:HIS:NE2  | 1:B:26:TYR:HB3  | 0.48     | 2.24        | 4      | 1     |
| 1:A:41:LEU:O    | 1:A:45:LEU:N    | 0.48     | 2.34        | 5      | 1     |
| 1:A:52:ASP:OD1  | 1:A:56:LYS:NZ   | 0.48     | 2.40        | 10     | 6     |
| 1:B:45:LEU:O    | 1:B:49:LYS:N    | 0.48     | 2.46        | 6      | 1     |
| 1:A:59:LYS:NZ   | 1:A:62:ASP:OD2  | 0.48     | 2.43        | 18     | 1     |
| 1:B:27:LYS:NZ   | 1:B:73:GLU:OE2  | 0.48     | 2.44        | 19     | 1     |
| 1:A:27:LYS:NZ   | 1:A:70:ASP:OD2  | 0.48     | 2.45        | 1      | 1     |
| 1:A:33:LEU:C    | 1:A:33:LEU:CD1  | 0.48     | 2.85        | 16     | 11    |
| 1:B:82:THR:O    | 1:B:86:ASN:N    | 0.48     | 2.44        | 7      | 6     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:30:LYS:NZ   | 1:B:62:ASP:OD1  | 0.48     | 2.44        | 11     | 3     |
| 1:A:4:LEU:N     | 1:A:4:LEU:CD2   | 0.48     | 2.76        | 12     | 2     |
| 1:B:27:LYS:NZ   | 1:B:68:GLU:OE1  | 0.48     | 2.40        | 4      | 3     |
| 1:B:59:LYS:HZ2  | 1:B:59:LYS:HB2  | 0.48     | 1.69        | 10     | 2     |
| 1:A:4:LEU:HD11  | 1:B:11:LEU:HD13 | 0.48     | 1.85        | 17     | 1     |
| 1:B:2:SER:C     | 1:B:4:LEU:N     | 0.48     | 2.72        | 16     | 6     |
| 1:B:47:ALA:HB3  | 1:B:85:MET:CG   | 0.48     | 2.39        | 9      | 1     |
| 1:A:56:LYS:O    | 1:A:60:GLU:N    | 0.48     | 2.46        | 17     | 1     |
| 1:A:40:GLU:CB   | 1:B:4:LEU:HD12  | 0.48     | 2.37        | 19     | 1     |
| 1:B:35:GLU:O    | 1:B:39:THR:OG1  | 0.47     | 2.31        | 5      | 9     |
| 1:B:18:HIS:ND1  | 1:B:32:GLU:OE1  | 0.47     | 2.47        | 15     | 3     |
| 1:B:76:VAL:O    | 1:B:80:ALA:N    | 0.47     | 2.39        | 14     | 7     |
| 1:B:55:ASP:HA   | 1:B:58:MET:HE2  | 0.47     | 1.85        | 9      | 1     |
| 1:A:30:LYS:CE   | 1:A:62:ASP:HA   | 0.47     | 2.39        | 11     | 1     |
| 1:A:37:LEU:HD12 | 1:A:77:LEU:HD21 | 0.47     | 1.84        | 13     | 1     |
| 1:A:30:LYS:CD   | 1:A:69:VAL:HB   | 0.47     | 2.39        | 2      | 3     |
| 1:A:55:ASP:OD2  | 1:A:59:LYS:NZ   | 0.47     | 2.41        | 10     | 3     |
| 1:B:34:LYS:HB2  | 1:B:34:LYS:HZ3  | 0.47     | 1.69        | 9      | 1     |
| 1:A:37:LEU:CD2  | 1:A:37:LEU:C    | 0.47     | 2.86        | 13     | 1     |
| 1:B:56:LYS:N    | 1:B:56:LYS:HD2  | 0.47     | 2.23        | 17     | 2     |
| 1:A:6:THR:O     | 1:A:10:THR:N    | 0.47     | 2.42        | 13     | 6     |
| 1:A:54:VAL:O    | 1:A:58:MET:HG2  | 0.47     | 2.09        | 12     | 2     |
| 1:A:51:VAL:C    | 1:A:53:ALA:H    | 0.47     | 2.17        | 5      | 3     |
| 1:B:61:LEU:CD2  | 1:B:77:LEU:HD13 | 0.47     | 2.40        | 9      | 1     |
| 1:B:61:LEU:HD23 | 1:B:77:LEU:HD13 | 0.47     | 1.85        | 9      | 1     |
| 1:B:71:PHE:CE2  | 1:B:75:VAL:HG11 | 0.47     | 2.44        | 10     | 2     |
| 1:B:34:LYS:NZ   | 1:B:35:GLU:OE2  | 0.47     | 2.44        | 13     | 1     |
| 1:B:15:PHE:CE2  | 1:B:28:LEU:HB3  | 0.47     | 2.44        | 20     | 1     |
| 1:B:61:LEU:O    | 1:B:64:ASN:HB3  | 0.47     | 2.09        | 5      | 2     |
| 1:B:64:ASN:ND2  | 1:B:68:GLU:O    | 0.47     | 2.44        | 5      | 1     |
| 1:A:72:GLN:HE21 | 1:B:83:VAL:HG11 | 0.47     | 1.69        | 11     | 1     |
| 1:B:49:LYS:O    | 1:B:49:LYS:NZ   | 0.47     | 2.42        | 11     | 1     |
| 1:A:48:GLN:HE21 | 1:A:48:GLN:C    | 0.47     | 2.17        | 2      | 1     |
| 1:B:4:LEU:HD22  | 1:B:4:LEU:N     | 0.47     | 2.23        | 5      | 1     |
| 1:B:58:MET:HG3  | 1:B:59:LYS:N    | 0.47     | 2.23        | 12     | 1     |
| 1:A:4:LEU:O     | 1:A:8:MET:HG2   | 0.47     | 2.09        | 14     | 6     |
| 1:A:87:ASN:HA   | 1:A:90:TRP:CE3  | 0.47     | 2.45        | 10     | 3     |
| 1:B:64:ASN:ND2  | 1:B:73:GLU:CD   | 0.47     | 2.72        | 20     | 2     |
| 1:A:90:TRP:CZ3  | 1:B:16:HIS:CG   | 0.47     | 3.03        | 12     | 1     |
| 1:A:28:LEU:N    | 1:A:69:VAL:O    | 0.47     | 2.46        | 1      | 2     |
| 1:A:62:ASP:O    | 1:A:65:GLY:N    | 0.47     | 2.43        | 16     | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:57:VAL:CG1  | 1:B:77:LEU:HD12 | 0.47     | 2.36        | 6      | 8     |
| 1:A:28:LEU:CD2  | 1:A:36:LEU:HD23 | 0.47     | 2.39        | 6      | 1     |
| 1:A:25:LYS:HB3  | 1:A:26:TYR:CD2  | 0.47     | 2.43        | 11     | 1     |
| 1:B:44:PHE:O    | 1:B:48:GLN:CG   | 0.47     | 2.63        | 13     | 1     |
| 1:A:89:PHE:N    | 1:A:89:PHE:CD1  | 0.47     | 2.82        | 18     | 1     |
| 1:A:8:MET:HE2   | 1:B:79:ALA:HA   | 0.47     | 1.86        | 9      | 1     |
| 1:B:54:VAL:HA   | 1:B:81:LEU:HD21 | 0.47     | 1.86        | 9      | 1     |
| 1:A:79:ALA:HB2  | 1:B:75:VAL:HG21 | 0.47     | 1.85        | 8      | 4     |
| 1:B:70:ASP:O    | 1:B:74:TYR:N    | 0.47     | 2.45        | 16     | 3     |
| 1:A:90:TRP:CZ2  | 1:B:12:ILE:HD12 | 0.47     | 2.45        | 9      | 1     |
| 1:B:44:PHE:O    | 1:B:48:GLN:NE2  | 0.47     | 2.48        | 17     | 2     |
| 1:A:55:ASP:HA   | 1:A:58:MET:SD   | 0.47     | 2.50        | 20     | 1     |
| 1:B:35:GLU:O    | 1:B:39:THR:CB   | 0.47     | 2.63        | 3      | 1     |
| 1:B:87:ASN:C    | 1:B:87:ASN:ND2  | 0.47     | 2.73        | 13     | 2     |
| 1:A:53:ALA:O    | 1:A:57:VAL:N    | 0.47     | 2.43        | 17     | 1     |
| 1:B:28:LEU:HD21 | 1:B:33:LEU:HD23 | 0.46     | 1.87        | 6      | 4     |
| 1:B:25:LYS:HB3  | 1:B:26:TYR:CE2  | 0.46     | 2.45        | 5      | 1     |
| 1:A:24:ASP:O    | 1:A:25:LYS:C    | 0.46     | 2.57        | 15     | 1     |
| 1:A:37:LEU:C    | 1:A:37:LEU:CD1  | 0.46     | 2.87        | 3      | 7     |
| 1:B:54:VAL:CG1  | 1:B:55:ASP:N    | 0.46     | 2.78        | 20     | 2     |
| 1:A:30:LYS:NZ   | 1:A:62:ASP:OD1  | 0.46     | 2.43        | 4      | 5     |
| 1:B:9:GLU:O     | 1:B:13:ASN:N    | 0.46     | 2.39        | 18     | 2     |
| 1:B:51:VAL:O    | 1:B:51:VAL:HG12 | 0.46     | 2.11        | 12     | 1     |
| 1:A:90:TRP:CE3  | 1:B:25:LYS:O    | 0.46     | 2.68        | 18     | 1     |
| 1:A:82:THR:HG21 | 1:B:8:MET:HB3   | 0.46     | 1.86        | 19     | 2     |
| 1:B:59:LYS:NZ   | 1:B:62:ASP:OD2  | 0.46     | 2.45        | 3      | 4     |
| 1:A:28:LEU:HB3  | 1:A:69:VAL:HG13 | 0.46     | 1.87        | 13     | 2     |
| 1:A:8:MET:SD    | 1:B:78:VAL:HB   | 0.46     | 2.50        | 4      | 1     |
| 1:A:55:ASP:O    | 1:A:59:LYS:HB2  | 0.46     | 2.11        | 20     | 1     |
| 1:B:64:ASN:C    | 1:B:66:ASP:N    | 0.46     | 2.72        | 5      | 3     |
| 1:B:30:LYS:NZ   | 1:B:64:ASN:C    | 0.46     | 2.74        | 7      | 1     |
| 1:A:48:GLN:NE2  | 1:A:54:VAL:HB   | 0.46     | 2.25        | 1      | 1     |
| 1:A:4:LEU:HD21  | 1:B:14:VAL:CG2  | 0.46     | 2.38        | 4      | 2     |
| 1:A:44:PHE:CE1  | 1:A:85:MET:HE2  | 0.46     | 2.45        | 9      | 4     |
| 1:B:45:LEU:O    | 1:B:49:LYS:HB2  | 0.46     | 2.10        | 12     | 1     |
| 1:A:8:MET:SD    | 1:B:78:VAL:CG2  | 0.46     | 3.04        | 4      | 1     |
| 1:A:36:LEU:HD12 | 1:A:36:LEU:O    | 0.46     | 2.10        | 9      | 2     |
| 1:A:33:LEU:HD21 | 1:A:77:LEU:HD22 | 0.46     | 1.88        | 16     | 1     |
| 1:A:41:LEU:N    | 1:A:41:LEU:HD12 | 0.46     | 2.26        | 17     | 2     |
| 1:A:4:LEU:HD22  | 1:B:14:VAL:HG21 | 0.46     | 1.86        | 17     | 1     |
| 1:A:27:LYS:CE   | 1:A:70:ASP:HB3  | 0.46     | 2.40        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:4:LEU:HD11  | 1:B:14:VAL:HG21 | 0.46     | 1.87        | 7      | 4     |
| 1:A:61:LEU:HD11 | 1:A:77:LEU:HB2  | 0.46     | 1.86        | 2      | 1     |
| 1:A:44:PHE:O    | 1:A:48:GLN:NE2  | 0.46     | 2.47        | 3      | 2     |
| 1:B:73:GLU:O    | 1:B:76:VAL:HG12 | 0.46     | 2.11        | 17     | 4     |
| 1:A:36:LEU:HG   | 1:A:37:LEU:N    | 0.46     | 2.25        | 20     | 4     |
| 1:A:26:TYR:O    | 1:A:26:TYR:CD2  | 0.46     | 2.69        | 18     | 2     |
| 1:B:3:GLU:H     | 1:B:3:GLU:CD    | 0.45     | 2.18        | 12     | 4     |
| 1:A:25:LYS:HE3  | 1:A:26:TYR:CZ   | 0.45     | 2.46        | 10     | 1     |
| 1:B:44:PHE:O    | 1:B:48:GLN:HG2  | 0.45     | 2.11        | 13     | 1     |
| 1:A:82:THR:OG1  | 1:B:8:MET:SD    | 0.45     | 2.74        | 17     | 1     |
| 1:B:25:LYS:H    | 1:B:25:LYS:HD3  | 0.45     | 1.71        | 6      | 1     |
| 1:A:90:TRP:HZ2  | 1:B:12:ILE:HG23 | 0.45     | 1.70        | 17     | 2     |
| 1:A:48:GLN:NE2  | 1:A:51:VAL:HG21 | 0.45     | 2.26        | 6      | 1     |
| 1:B:28:LEU:N    | 1:B:69:VAL:O    | 0.45     | 2.47        | 12     | 1     |
| 1:A:90:TRP:CE2  | 1:B:16:HIS:ND1  | 0.45     | 2.85        | 4      | 2     |
| 1:B:47:ALA:HB1  | 1:B:85:MET:HE3  | 0.45     | 1.87        | 9      | 1     |
| 1:A:36:LEU:C    | 1:A:36:LEU:CD1  | 0.45     | 2.89        | 17     | 3     |
| 1:A:3:GLU:O     | 1:A:7:ALA:N     | 0.45     | 2.38        | 13     | 8     |
| 1:B:28:LEU:HD11 | 1:B:32:GLU:HB2  | 0.45     | 1.87        | 5      | 2     |
| 1:B:22:GLU:OE1  | 1:B:23:GLY:N    | 0.45     | 2.50        | 8      | 2     |
| 1:A:30:LYS:NZ   | 1:A:73:GLU:OE1  | 0.45     | 2.44        | 14     | 2     |
| 1:A:90:TRP:CZ2  | 1:B:12:ILE:HG23 | 0.45     | 2.47        | 17     | 2     |
| 1:A:12:ILE:HD13 | 1:A:71:PHE:CE1  | 0.45     | 2.47        | 9      | 4     |
| 1:B:9:GLU:O     | 1:B:13:ASN:ND2  | 0.45     | 2.49        | 4      | 5     |
| 1:A:34:LYS:CG   | 1:A:35:GLU:N    | 0.45     | 2.78        | 8      | 1     |
| 1:A:61:LEU:HG   | 1:A:77:LEU:HB2  | 0.45     | 1.88        | 12     | 1     |
| 1:A:87:ASN:C    | 1:A:87:ASN:ND2  | 0.45     | 2.75        | 12     | 1     |
| 1:A:18:HIS:HB3  | 1:A:28:LEU:CD1  | 0.45     | 2.42        | 20     | 1     |
| 1:A:70:ASP:N    | 1:A:73:GLU:OE1  | 0.45     | 2.49        | 1      | 1     |
| 1:B:32:GLU:O    | 1:B:36:LEU:HB3  | 0.45     | 2.12        | 18     | 7     |
| 1:A:3:GLU:H     | 1:A:3:GLU:CD    | 0.45     | 2.20        | 17     | 3     |
| 1:A:79:ALA:HB2  | 1:B:75:VAL:HG11 | 0.45     | 1.88        | 16     | 3     |
| 1:A:25:LYS:NZ   | 1:A:26:TYR:OH   | 0.45     | 2.35        | 8      | 3     |
| 1:A:86:ASN:O    | 1:A:89:PHE:HB2  | 0.44     | 2.12        | 10     | 2     |
| 1:A:2:SER:O     | 1:A:4:LEU:N     | 0.44     | 2.50        | 2      | 2     |
| 1:A:25:LYS:C    | 1:A:26:TYR:CD1  | 0.44     | 2.95        | 2      | 1     |
| 1:B:17:ALA:O    | 1:B:21:LYS:NZ   | 0.44     | 2.41        | 3      | 1     |
| 1:A:78:VAL:CB   | 1:B:8:MET:SD    | 0.44     | 3.05        | 17     | 1     |
| 1:B:6:THR:O     | 1:B:10:THR:N    | 0.44     | 2.45        | 20     | 7     |
| 1:B:24:ASP:O    | 1:B:25:LYS:C    | 0.44     | 2.60        | 3      | 1     |
| 1:B:85:MET:O    | 1:B:89:PHE:N    | 0.44     | 2.50        | 4      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:26:TYR:CD1  | 1:A:26:TYR:N    | 0.44     | 2.83        | 6      | 1     |
| 1:A:34:LYS:HG3  | 1:A:35:GLU:N    | 0.44     | 2.27        | 6      | 2     |
| 1:B:55:ASP:CG   | 1:B:59:LYS:NZ   | 0.44     | 2.75        | 8      | 1     |
| 1:A:15:PHE:CE2  | 1:A:28:LEU:CB   | 0.44     | 3.00        | 17     | 2     |
| 1:B:34:LYS:HG3  | 1:B:35:GLU:N    | 0.44     | 2.27        | 3      | 1     |
| 1:A:4:LEU:HD22  | 1:A:4:LEU:N     | 0.44     | 2.27        | 11     | 3     |
| 1:A:61:LEU:CD2  | 1:A:61:LEU:N    | 0.44     | 2.80        | 7      | 1     |
| 1:A:63:GLU:C    | 1:A:65:GLY:H    | 0.44     | 2.19        | 19     | 2     |
| 1:A:25:LYS:CB   | 1:A:26:TYR:CD2  | 0.44     | 3.00        | 11     | 1     |
| 1:B:70:ASP:N    | 1:B:73:GLU:OE1  | 0.44     | 2.47        | 12     | 1     |
| 1:B:26:TYR:CD1  | 1:B:26:TYR:N    | 0.44     | 2.85        | 16     | 1     |
| 1:B:61:LEU:CG   | 1:B:77:LEU:HD13 | 0.44     | 2.40        | 11     | 4     |
| 1:A:90:TRP:CE2  | 1:B:16:HIS:CE1  | 0.44     | 3.05        | 4      | 1     |
| 1:B:25:LYS:HD2  | 1:B:26:TYR:CZ   | 0.44     | 2.47        | 8      | 1     |
| 1:B:12:ILE:O    | 1:B:16:HIS:N    | 0.44     | 2.37        | 12     | 3     |
| 1:A:27:LYS:HZ3  | 1:A:70:ASP:HB2  | 0.44     | 1.71        | 12     | 1     |
| 1:A:47:ALA:HB1  | 1:A:85:MET:SD   | 0.44     | 2.52        | 17     | 1     |
| 1:B:55:ASP:OD2  | 1:B:56:LYS:NZ   | 0.44     | 2.48        | 17     | 1     |
| 1:A:45:LEU:O    | 1:A:49:LYS:N    | 0.44     | 2.50        | 12     | 1     |
| 1:A:49:LYS:O    | 1:A:49:LYS:NZ   | 0.44     | 2.45        | 12     | 1     |
| 1:A:86:ASN:HD22 | 1:B:12:ILE:HG13 | 0.44     | 1.73        | 12     | 2     |
| 1:A:44:PHE:O    | 1:A:48:GLN:N    | 0.44     | 2.45        | 18     | 1     |
| 1:A:44:PHE:O    | 1:A:48:GLN:HG3  | 0.44     | 2.11        | 7      | 3     |
| 1:B:12:ILE:CG2  | 1:B:16:HIS:NE2  | 0.44     | 2.80        | 6      | 1     |
| 1:A:18:HIS:ND1  | 1:A:32:GLU:OE1  | 0.44     | 2.47        | 17     | 3     |
| 1:A:80:ALA:CB   | 1:B:72:GLN:HE21 | 0.44     | 2.25        | 8      | 1     |
| 1:B:19:SER:OG   | 1:B:27:LYS:O    | 0.44     | 2.35        | 20     | 2     |
| 1:A:48:GLN:HE22 | 1:A:54:VAL:HG23 | 0.44     | 1.72        | 16     | 1     |
| 1:B:28:LEU:O    | 1:B:69:VAL:HG12 | 0.44     | 2.13        | 6      | 2     |
| 1:B:37:LEU:HD22 | 1:B:37:LEU:C    | 0.44     | 2.37        | 3      | 1     |
| 1:A:90:TRP:NE1  | 1:B:16:HIS:HE2  | 0.44     | 2.10        | 9      | 1     |
| 1:A:25:LYS:HD2  | 1:A:26:TYR:CE2  | 0.44     | 2.47        | 10     | 1     |
| 1:B:3:GLU:OE1   | 1:B:3:GLU:N     | 0.44     | 2.44        | 13     | 1     |
| 1:A:90:TRP:CE2  | 1:B:16:HIS:NE2  | 0.44     | 2.85        | 14     | 1     |
| 1:A:44:PHE:CD2  | 1:A:85:MET:HE2  | 0.44     | 2.48        | 15     | 1     |
| 1:A:9:GLU:O     | 1:A:13:ASN:N    | 0.44     | 2.44        | 19     | 1     |
| 1:A:18:HIS:NE2  | 1:A:40:GLU:OE2  | 0.44     | 2.51        | 20     | 2     |
| 1:B:59:LYS:O    | 1:B:63:GLU:HG2  | 0.44     | 2.13        | 7      | 2     |
| 1:B:37:LEU:HD22 | 1:B:41:LEU:HB2  | 0.44     | 1.89        | 4      | 1     |
| 1:A:90:TRP:CE3  | 1:B:26:TYR:CB   | 0.44     | 3.00        | 9      | 1     |
| 1:A:48:GLN:O    | 1:A:54:VAL:HG11 | 0.44     | 2.13        | 13     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:85:MET:O    | 1:A:88:PHE:HB3  | 0.44     | 2.13        | 15     | 1     |
| 1:A:26:TYR:OH   | 1:B:87:ASN:ND2  | 0.44     | 2.39        | 6      | 1     |
| 1:A:44:PHE:O    | 1:A:48:GLN:CG   | 0.44     | 2.66        | 7      | 1     |
| 1:A:26:TYR:O    | 1:A:27:LYS:HG2  | 0.44     | 2.13        | 8      | 3     |
| 1:A:18:HIS:NE2  | 1:A:36:LEU:HB2  | 0.44     | 2.28        | 14     | 2     |
| 1:A:90:TRP:N    | 1:A:90:TRP:HD1  | 0.44     | 2.10        | 19     | 1     |
| 1:A:37:LEU:HD11 | 1:A:81:LEU:HD11 | 0.43     | 1.88        | 1      | 2     |
| 1:B:54:VAL:O    | 1:B:58:MET:CG   | 0.43     | 2.66        | 2      | 1     |
| 1:A:38:GLN:HB2  | 1:A:45:LEU:CD2  | 0.43     | 2.43        | 3      | 1     |
| 1:B:24:ASP:O    | 1:B:26:TYR:N    | 0.43     | 2.51        | 3      | 1     |
| 1:A:54:VAL:O    | 1:A:58:MET:CB   | 0.43     | 2.66        | 7      | 2     |
| 1:B:19:SER:HA   | 1:B:27:LYS:O    | 0.43     | 2.13        | 9      | 1     |
| 1:A:75:VAL:HG11 | 1:B:79:ALA:HB2  | 0.43     | 1.90        | 16     | 1     |
| 1:A:3:GLU:CD    | 1:A:3:GLU:H     | 0.43     | 2.17        | 18     | 1     |
| 1:A:8:MET:SD    | 1:B:78:VAL:C    | 0.43     | 3.01        | 4      | 2     |
| 1:B:26:TYR:O    | 1:B:27:LYS:HG2  | 0.43     | 2.14        | 15     | 4     |
| 1:B:60:GLU:O    | 1:B:64:ASN:N    | 0.43     | 2.42        | 10     | 1     |
| 1:A:59:LYS:O    | 1:A:63:GLU:HG2  | 0.43     | 2.13        | 13     | 3     |
| 1:B:34:LYS:NZ   | 1:B:34:LYS:HB3  | 0.43     | 2.28        | 11     | 1     |
| 1:A:12:ILE:HG21 | 1:B:86:ASN:CG   | 0.43     | 2.38        | 17     | 1     |
| 1:B:48:GLN:NE2  | 1:B:51:VAL:HB   | 0.43     | 2.28        | 18     | 2     |
| 1:A:4:LEU:O     | 1:A:8:MET:N     | 0.43     | 2.40        | 19     | 1     |
| 1:A:90:TRP:CE3  | 1:B:26:TYR:HB3  | 0.43     | 2.47        | 19     | 1     |
| 1:A:34:LYS:HZ2  | 1:A:34:LYS:CB   | 0.43     | 2.25        | 4      | 1     |
| 1:A:90:TRP:CE3  | 1:B:16:HIS:CD2  | 0.43     | 3.06        | 7      | 1     |
| 1:B:82:THR:O    | 1:B:86:ASN:HB2  | 0.43     | 2.12        | 18     | 1     |
| 1:A:36:LEU:HD12 | 1:A:40:GLU:CD   | 0.43     | 2.38        | 1      | 1     |
| 1:B:44:PHE:O    | 1:B:48:GLN:HG3  | 0.43     | 2.13        | 14     | 2     |
| 1:A:64:ASN:O    | 1:A:64:ASN:CG   | 0.43     | 2.61        | 3      | 1     |
| 1:A:71:PHE:CE2  | 1:A:75:VAL:HG11 | 0.43     | 2.48        | 9      | 2     |
| 1:A:16:HIS:CE1  | 1:A:26:TYR:CD2  | 0.43     | 3.07        | 4      | 1     |
| 1:A:90:TRP:CZ2  | 1:B:16:HIS:NE2  | 0.43     | 2.86        | 8      | 2     |
| 1:A:56:LYS:N    | 1:A:56:LYS:HD2  | 0.43     | 2.28        | 9      | 1     |
| 1:B:2:SER:O     | 1:B:5:GLU:N     | 0.43     | 2.52        | 13     | 2     |
| 1:A:36:LEU:HD12 | 1:A:40:GLU:CG   | 0.43     | 2.43        | 12     | 1     |
| 1:A:61:LEU:HG   | 1:A:77:LEU:CD1  | 0.43     | 2.42        | 14     | 1     |
| 1:B:17:ALA:O    | 1:B:21:LYS:HG2  | 0.43     | 2.13        | 1      | 3     |
| 1:B:18:HIS:NE2  | 1:B:36:LEU:HD13 | 0.43     | 2.27        | 8      | 2     |
| 1:B:22:GLU:OE1  | 1:B:31:LYS:NZ   | 0.43     | 2.44        | 3      | 1     |
| 1:B:68:GLU:OE1  | 1:B:68:GLU:N    | 0.43     | 2.51        | 5      | 1     |
| 1:B:28:LEU:O    | 1:B:69:VAL:CG1  | 0.43     | 2.66        | 9      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:12:ILE:CG2  | 1:B:86:ASN:OD1  | 0.43     | 2.66        | 8      | 1     |
| 1:A:25:LYS:HB3  | 1:A:26:TYR:CE2  | 0.43     | 2.49        | 11     | 1     |
| 1:B:55:ASP:O    | 1:B:59:LYS:HB2  | 0.43     | 2.14        | 16     | 1     |
| 1:A:30:LYS:CG   | 1:A:65:GLY:HA2  | 0.43     | 2.43        | 17     | 1     |
| 1:A:44:PHE:CE2  | 1:A:82:THR:HG23 | 0.43     | 2.48        | 17     | 1     |
| 1:B:31:LYS:O    | 1:B:35:GLU:HG3  | 0.43     | 2.13        | 7      | 1     |
| 1:B:25:LYS:CG   | 1:B:26:TYR:H    | 0.43     | 2.25        | 9      | 1     |
| 1:B:22:GLU:C    | 1:B:22:GLU:CD   | 0.43     | 2.86        | 10     | 1     |
| 1:A:22:GLU:OE2  | 1:A:24:ASP:N    | 0.43     | 2.50        | 14     | 1     |
| 1:B:27:LYS:HZ3  | 1:B:70:ASP:HB3  | 0.43     | 1.74        | 14     | 1     |
| 1:A:36:LEU:O    | 1:A:36:LEU:HD12 | 0.43     | 2.14        | 6      | 2     |
| 1:B:61:LEU:N    | 1:B:61:LEU:CD2  | 0.43     | 2.82        | 8      | 3     |
| 1:A:75:VAL:HG21 | 1:B:79:ALA:HB3  | 0.43     | 1.90        | 14     | 2     |
| 1:B:59:LYS:HG2  | 1:B:60:GLU:N    | 0.43     | 2.28        | 15     | 1     |
| 1:A:73:GLU:O    | 1:A:76:VAL:HG12 | 0.43     | 2.14        | 2      | 3     |
| 1:A:54:VAL:O    | 1:A:58:MET:N    | 0.43     | 2.42        | 7      | 1     |
| 1:A:86:ASN:ND2  | 1:B:12:ILE:HG21 | 0.43     | 2.29        | 8      | 1     |
| 1:B:30:LYS:NZ   | 1:B:65:GLY:N    | 0.43     | 2.67        | 4      | 1     |
| 1:A:54:VAL:HG23 | 1:A:81:LEU:HD21 | 0.43     | 1.91        | 6      | 1     |
| 1:A:34:LYS:NZ   | 1:A:62:ASP:CG   | 0.43     | 2.77        | 14     | 1     |
| 1:A:38:GLN:O    | 1:A:42:SER:OG   | 0.43     | 2.35        | 16     | 1     |
| 1:A:85:MET:HE3  | 1:A:89:PHE:CE1  | 0.43     | 2.49        | 17     | 1     |
| 1:B:25:LYS:C    | 1:B:26:TYR:CD1  | 0.43     | 2.97        | 18     | 1     |
| 1:B:46:ASP:HA   | 1:B:49:LYS:HZ3  | 0.43     | 1.73        | 2      | 1     |
| 1:B:30:LYS:NZ   | 1:B:65:GLY:HA2  | 0.43     | 2.28        | 18     | 2     |
| 1:B:83:VAL:O    | 1:B:87:ASN:N    | 0.43     | 2.49        | 18     | 2     |
| 1:A:17:ALA:O    | 1:A:21:LYS:HG2  | 0.43     | 2.14        | 11     | 2     |
| 1:A:21:LYS:HA   | 1:A:21:LYS:HZ3  | 0.43     | 1.74        | 20     | 1     |
| 1:B:44:PHE:CD1  | 1:B:85:MET:CE   | 0.42     | 3.02        | 18     | 2     |
| 1:A:42:SER:O    | 1:A:46:ASP:N    | 0.42     | 2.46        | 16     | 2     |
| 1:B:82:THR:O    | 1:B:86:ASN:CB   | 0.42     | 2.67        | 17     | 2     |
| 1:A:90:TRP:CD1  | 1:B:16:HIS:CE1  | 0.42     | 3.07        | 5      | 1     |
| 1:B:88:PHE:O    | 1:B:89:PHE:C    | 0.42     | 2.62        | 16     | 2     |
| 1:B:15:PHE:CZ   | 1:B:71:PHE:N    | 0.42     | 2.87        | 13     | 1     |
| 1:B:25:LYS:HD2  | 1:B:26:TYR:CE1  | 0.42     | 2.49        | 7      | 1     |
| 1:A:59:LYS:NZ   | 1:A:63:GLU:OE1  | 0.42     | 2.44        | 8      | 1     |
| 1:A:25:LYS:CE   | 1:A:26:TYR:CZ   | 0.42     | 3.03        | 10     | 1     |
| 1:B:48:GLN:NE2  | 1:B:54:VAL:HB   | 0.42     | 2.29        | 18     | 2     |
| 1:A:45:LEU:HD13 | 1:A:58:MET:CE   | 0.42     | 2.43        | 17     | 1     |
| 1:A:78:VAL:HG23 | 1:B:8:MET:HE2   | 0.42     | 1.89        | 7      | 3     |
| 1:A:52:ASP:O    | 1:A:55:ASP:N    | 0.42     | 2.52        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:82:THR:O    | 1:A:86:ASN:HB2  | 0.42     | 2.14        | 10     | 1     |
| 1:A:90:TRP:CZ3  | 1:B:16:HIS:CE1  | 0.42     | 3.07        | 18     | 1     |
| 1:A:41:LEU:O    | 1:A:45:LEU:CB   | 0.42     | 2.68        | 5      | 1     |
| 1:B:51:VAL:C    | 1:B:53:ALA:N    | 0.42     | 2.77        | 13     | 3     |
| 1:A:2:SER:C     | 1:A:4:LEU:H     | 0.42     | 2.21        | 15     | 2     |
| 1:A:31:LYS:CG   | 1:A:32:GLU:N    | 0.42     | 2.82        | 13     | 1     |
| 1:A:27:LYS:NZ   | 1:A:68:GLU:OE2  | 0.42     | 2.46        | 18     | 1     |
| 1:A:22:GLU:OE1  | 1:A:28:LEU:HD12 | 0.42     | 2.14        | 4      | 1     |
| 1:A:26:TYR:CZ   | 1:B:87:ASN:OD1  | 0.42     | 2.73        | 5      | 1     |
| 1:B:35:GLU:O    | 1:B:38:GLN:HG2  | 0.42     | 2.13        | 18     | 1     |
| 1:A:61:LEU:N    | 1:A:61:LEU:CD2  | 0.42     | 2.82        | 16     | 6     |
| 1:A:40:GLU:O    | 1:B:2:SER:OG    | 0.42     | 2.33        | 8      | 2     |
| 1:A:59:LYS:O    | 1:A:62:ASP:N    | 0.42     | 2.53        | 7      | 1     |
| 1:A:59:LYS:NZ   | 1:A:59:LYS:O    | 0.42     | 2.37        | 14     | 2     |
| 1:A:43:GLY:N    | 1:B:5:GLU:OE2   | 0.42     | 2.50        | 7      | 1     |
| 1:A:83:VAL:O    | 1:A:87:ASN:N    | 0.42     | 2.52        | 7      | 1     |
| 1:A:38:GLN:CB   | 1:A:45:LEU:HD22 | 0.42     | 2.44        | 8      | 1     |
| 1:A:4:LEU:N     | 1:A:4:LEU:HD23  | 0.42     | 2.29        | 19     | 1     |
| 1:A:34:LYS:HB2  | 1:A:34:LYS:NZ   | 0.42     | 2.22        | 4      | 1     |
| 1:A:61:LEU:HD12 | 1:A:77:LEU:HD22 | 0.42     | 1.90        | 5      | 1     |
| 1:B:44:PHE:C    | 1:B:48:GLN:NE2  | 0.42     | 2.78        | 10     | 1     |
| 1:B:36:LEU:C    | 1:B:36:LEU:CD1  | 0.42     | 2.91        | 13     | 1     |
| 1:A:32:GLU:O    | 1:A:36:LEU:HB3  | 0.42     | 2.15        | 20     | 1     |
| 1:A:6:THR:O     | 1:A:10:THR:OG1  | 0.42     | 2.36        | 8      | 3     |
| 1:B:29:SER:HB2  | 1:B:31:LYS:HG3  | 0.42     | 1.89        | 5      | 1     |
| 1:A:19:SER:HA   | 1:A:27:LYS:O    | 0.42     | 2.14        | 12     | 2     |
| 1:B:15:PHE:CE1  | 1:B:28:LEU:CB   | 0.42     | 3.02        | 13     | 2     |
| 1:B:28:LEU:HD21 | 1:B:36:LEU:HD23 | 0.42     | 1.90        | 8      | 2     |
| 1:A:50:ASP:C    | 1:A:52:ASP:N    | 0.42     | 2.78        | 9      | 1     |
| 1:B:48:GLN:OE1  | 1:B:81:LEU:HB3  | 0.42     | 2.15        | 10     | 1     |
| 1:A:22:GLU:OE1  | 1:A:23:GLY:N    | 0.42     | 2.50        | 15     | 1     |
| 1:B:44:PHE:CE2  | 1:B:85:MET:CE   | 0.42     | 3.01        | 20     | 1     |
| 1:A:62:ASP:C    | 1:A:65:GLY:H    | 0.41     | 2.23        | 2      | 1     |
| 1:A:60:GLU:O    | 1:A:64:ASN:N    | 0.41     | 2.39        | 5      | 1     |
| 1:B:28:LEU:HB3  | 1:B:69:VAL:O    | 0.41     | 2.15        | 7      | 1     |
| 1:A:47:ALA:HB3  | 1:A:85:MET:HG3  | 0.41     | 1.92        | 12     | 2     |
| 1:A:8:MET:CE    | 1:B:79:ALA:HA   | 0.41     | 2.45        | 9      | 1     |
| 1:A:4:LEU:CD1   | 1:B:11:LEU:CD2  | 0.41     | 2.91        | 1      | 1     |
| 1:B:4:LEU:O     | 1:B:8:MET:HG2   | 0.41     | 2.14        | 1      | 2     |
| 1:A:40:GLU:O    | 1:B:2:SER:N     | 0.41     | 2.44        | 12     | 1     |
| 1:A:71:PHE:O    | 1:A:75:VAL:HG13 | 0.41     | 2.15        | 13     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:64:ASN:ND2  | 1:B:73:GLU:OE1  | 0.41     | 2.52        | 16     | 1     |
| 1:B:45:LEU:O    | 1:B:45:LEU:HD12 | 0.41     | 2.15        | 19     | 1     |
| 1:A:74:TYR:OH   | 1:B:4:LEU:HD13  | 0.41     | 2.15        | 2      | 1     |
| 1:A:83:VAL:CG2  | 1:A:87:ASN:ND2  | 0.41     | 2.83        | 2      | 1     |
| 1:A:72:GLN:O    | 1:A:75:VAL:HG22 | 0.41     | 2.16        | 7      | 1     |
| 1:A:18:HIS:O    | 1:A:21:LYS:N    | 0.41     | 2.53        | 20     | 1     |
| 1:B:49:LYS:NZ   | 1:B:50:ASP:OD1  | 0.41     | 2.42        | 3      | 1     |
| 1:B:30:LYS:N    | 1:B:30:LYS:HD2  | 0.41     | 2.29        | 7      | 1     |
| 1:A:86:ASN:HB3  | 1:A:90:TRP:CE2  | 0.41     | 2.50        | 9      | 1     |
| 1:A:14:VAL:HG21 | 1:B:4:LEU:CD1   | 0.41     | 2.31        | 13     | 2     |
| 1:B:48:GLN:NE2  | 1:B:54:VAL:HG21 | 0.41     | 2.30        | 13     | 1     |
| 1:A:19:SER:O    | 1:A:23:GLY:N    | 0.41     | 2.50        | 2      | 1     |
| 1:A:90:TRP:HE1  | 1:B:16:HIS:CE1  | 0.41     | 2.33        | 2      | 2     |
| 1:A:4:LEU:HD22  | 1:A:4:LEU:H     | 0.41     | 1.75        | 7      | 1     |
| 1:B:78:VAL:O    | 1:B:82:THR:OG1  | 0.41     | 2.35        | 14     | 1     |
| 1:A:57:VAL:HG22 | 1:A:80:ALA:CB   | 0.41     | 2.46        | 16     | 1     |
| 1:B:54:VAL:O    | 1:B:58:MET:HG2  | 0.41     | 2.16        | 16     | 1     |
| 1:B:4:LEU:H     | 1:B:4:LEU:HD22  | 0.41     | 1.74        | 1      | 1     |
| 1:B:59:LYS:O    | 1:B:62:ASP:HB2  | 0.41     | 2.15        | 1      | 1     |
| 1:B:36:LEU:HG   | 1:B:37:LEU:N    | 0.41     | 2.30        | 6      | 4     |
| 1:B:25:LYS:HG3  | 1:B:26:TYR:CE1  | 0.41     | 2.50        | 4      | 1     |
| 1:A:48:GLN:CB   | 1:A:51:VAL:HG21 | 0.41     | 2.45        | 10     | 1     |
| 1:A:73:GLU:OE1  | 1:A:73:GLU:N    | 0.41     | 2.48        | 10     | 1     |
| 1:B:44:PHE:CE2  | 1:B:82:THR:HA   | 0.41     | 2.51        | 20     | 1     |
| 1:A:28:LEU:O    | 1:A:69:VAL:HG13 | 0.41     | 2.15        | 9      | 2     |
| 1:A:73:GLU:O    | 1:A:76:VAL:HG22 | 0.41     | 2.16        | 6      | 2     |
| 1:B:4:LEU:CD2   | 1:B:4:LEU:H     | 0.41     | 2.28        | 8      | 1     |
| 1:A:83:VAL:HG23 | 1:A:90:TRP:CH2  | 0.41     | 2.50        | 10     | 2     |
| 1:A:49:LYS:NZ   | 1:A:50:ASP:OD1  | 0.41     | 2.43        | 12     | 1     |
| 1:B:72:GLN:O    | 1:B:75:VAL:HG22 | 0.41     | 2.15        | 17     | 1     |
| 1:A:8:MET:SD    | 1:B:78:VAL:CB   | 0.41     | 3.09        | 4      | 1     |
| 1:B:36:LEU:CD1  | 1:B:40:GLU:CG   | 0.41     | 2.99        | 8      | 1     |
| 1:A:44:PHE:HD1  | 1:A:85:MET:SD   | 0.41     | 2.38        | 19     | 2     |
| 1:B:61:LEU:HG   | 1:B:77:LEU:HB2  | 0.41     | 1.93        | 11     | 1     |
| 1:B:73:GLU:HA   | 1:B:76:VAL:HG12 | 0.41     | 1.93        | 11     | 1     |
| 1:A:27:LYS:HZ3  | 1:A:70:ASP:CB   | 0.41     | 2.29        | 12     | 1     |
| 1:B:30:LYS:HE3  | 1:B:61:LEU:O    | 0.41     | 2.16        | 12     | 1     |
| 1:B:38:GLN:HG3  | 1:B:39:THR:N    | 0.41     | 2.31        | 20     | 1     |
| 1:B:61:LEU:O    | 1:B:64:ASN:C    | 0.41     | 2.63        | 1      | 1     |
| 1:A:48:GLN:NE2  | 1:A:54:VAL:HG23 | 0.41     | 2.31        | 2      | 1     |
| 1:B:63:GLU:C    | 1:B:65:GLY:N    | 0.41     | 2.79        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:18:HIS:ND1  | 1:B:32:GLU:HB3  | 0.41     | 2.31        | 6      | 2     |
| 1:A:5:GLU:OE2   | 1:B:43:GLY:N    | 0.41     | 2.54        | 12     | 1     |
| 1:A:50:ASP:OD1  | 1:A:50:ASP:N    | 0.41     | 2.54        | 16     | 1     |
| 1:B:42:SER:O    | 1:B:46:ASP:N    | 0.41     | 2.44        | 18     | 1     |
| 1:A:18:HIS:O    | 1:A:21:LYS:HB3  | 0.41     | 2.16        | 20     | 1     |
| 1:A:54:VAL:CG1  | 1:A:55:ASP:N    | 0.40     | 2.84        | 2      | 1     |
| 1:B:47:ALA:HB1  | 1:B:85:MET:SD   | 0.40     | 2.55        | 2      | 1     |
| 1:B:30:LYS:NZ   | 1:B:65:GLY:CA   | 0.40     | 2.84        | 4      | 1     |
| 1:A:80:ALA:HB2  | 1:B:72:GLN:NE2  | 0.40     | 2.31        | 6      | 1     |
| 1:A:30:LYS:CE   | 1:A:69:VAL:HB   | 0.40     | 2.46        | 13     | 1     |
| 1:A:31:LYS:HG3  | 1:A:32:GLU:N    | 0.40     | 2.31        | 13     | 1     |
| 1:A:78:VAL:O    | 1:A:82:THR:OG1  | 0.40     | 2.38        | 17     | 1     |
| 1:A:83:VAL:HG22 | 1:A:87:ASN:ND2  | 0.40     | 2.32        | 2      | 1     |
| 1:B:55:ASP:CG   | 1:B:59:LYS:HZ3  | 0.40     | 2.24        | 8      | 1     |
| 1:A:14:VAL:CG2  | 1:B:4:LEU:HD21  | 0.40     | 2.46        | 11     | 1     |
| 1:A:87:ASN:OD1  | 1:B:26:TYR:CE2  | 0.40     | 2.74        | 13     | 1     |
| 1:A:29:SER:C    | 1:A:31:LYS:N    | 0.40     | 2.79        | 1      | 1     |
| 1:A:86:ASN:ND2  | 1:B:9:GLU:OE2   | 0.40     | 2.43        | 4      | 1     |
| 1:A:44:PHE:O    | 1:A:48:GLN:HG2  | 0.40     | 2.16        | 5      | 1     |
| 1:A:61:LEU:HD23 | 1:A:77:LEU:HD13 | 0.40     | 1.92        | 7      | 1     |
| 1:B:12:ILE:HD13 | 1:B:71:PHE:CE1  | 0.40     | 2.52        | 9      | 1     |
| 1:A:25:LYS:HE2  | 1:A:26:TYR:CZ   | 0.40     | 2.50        | 18     | 2     |
| 1:A:87:ASN:OD1  | 1:B:26:TYR:CZ   | 0.40     | 2.74        | 20     | 1     |
| 1:B:19:SER:CB   | 1:B:27:LYS:O    | 0.40     | 2.70        | 20     | 1     |
| 1:A:27:LYS:HD2  | 1:A:70:ASP:HB3  | 0.40     | 1.94        | 1      | 1     |
| 1:B:22:GLU:OE1  | 1:B:31:LYS:HE3  | 0.40     | 2.17        | 2      | 1     |
| 1:B:45:LEU:O    | 1:B:49:LYS:HG3  | 0.40     | 2.16        | 4      | 1     |
| 1:A:34:LYS:HB3  | 1:A:34:LYS:NZ   | 0.40     | 2.31        | 19     | 1     |
| 1:B:21:LYS:NZ   | 1:B:32:GLU:OE1  | 0.40     | 2.52        | 2      | 1     |
| 1:A:55:ASP:O    | 1:A:58:MET:HB2  | 0.40     | 2.17        | 3      | 1     |
| 1:B:70:ASP:OD1  | 1:B:71:PHE:N    | 0.40     | 2.52        | 4      | 1     |
| 1:A:26:TYR:CD1  | 1:A:26:TYR:O    | 0.40     | 2.75        | 9      | 1     |
| 1:A:86:ASN:O    | 1:A:87:ASN:C    | 0.40     | 2.65        | 16     | 1     |
| 1:A:48:GLN:NE2  | 1:A:54:VAL:HG11 | 0.40     | 2.31        | 17     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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     | 89/93 (96%)     | 83±1 (94±2%) | 5±2 (5±2%) | 1±1 (1±1%) | 13          | 61 |
| 1   | B     | 88/93 (95%)     | 82±2 (94±2%) | 4±1 (5±1%) | 1±1 (2±1%) | 11          | 57 |
| All | All   | 3540/3720 (95%) | 3316 (94%)   | 175 (5%)   | 49 (1%)    | 11          | 58 |

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 67  | GLY  | 12             |
| 1   | A     | 67  | GLY  | 8              |
| 1   | B     | 23  | GLY  | 5              |
| 1   | B     | 24  | ASP  | 3              |
| 1   | B     | 25  | LYS  | 3              |
| 1   | A     | 25  | LYS  | 3              |
| 1   | A     | 3   | GLU  | 2              |
| 1   | A     | 65  | GLY  | 2              |
| 1   | A     | 23  | GLY  | 2              |
| 1   | A     | 24  | ASP  | 2              |
| 1   | A     | 22  | GLU  | 1              |
| 1   | A     | 90  | TRP  | 1              |
| 1   | B     | 22  | GLU  | 1              |
| 1   | B     | 65  | GLY  | 1              |
| 1   | A     | 51  | VAL  | 1              |
| 1   | B     | 52  | ASP  | 1              |
| 1   | B     | 89  | PHE  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers    | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|-------------|----|
| 1   | A     | 77/80 (96%)     | 68±2 (89±2%) | 9±2 (11±2%) | 8           | 50 |
| 1   | B     | 76/80 (95%)     | 67±2 (88±3%) | 9±2 (12±3%) | 7           | 48 |
| All | All   | 3060/3200 (96%) | 2696 (88%)   | 364 (12%)   | 7           | 49 |

All 71 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     | 36  | LEU  | 17             |
| 1   | A     | 69  | VAL  | 15             |
| 1   | A     | 36  | LEU  | 15             |
| 1   | B     | 48  | GLN  | 14             |
| 1   | B     | 69  | VAL  | 14             |
| 1   | B     | 70  | ASP  | 14             |
| 1   | B     | 45  | LEU  | 14             |
| 1   | A     | 70  | ASP  | 14             |
| 1   | B     | 59  | LYS  | 13             |
| 1   | A     | 48  | GLN  | 11             |
| 1   | A     | 42  | SER  | 11             |
| 1   | B     | 26  | TYR  | 10             |
| 1   | A     | 59  | LYS  | 10             |
| 1   | A     | 4   | LEU  | 9              |
| 1   | A     | 22  | GLU  | 9              |
| 1   | A     | 25  | LYS  | 8              |
| 1   | A     | 26  | TYR  | 8              |
| 1   | A     | 30  | LYS  | 8              |
| 1   | B     | 29  | SER  | 8              |
| 1   | B     | 30  | LYS  | 8              |
| 1   | A     | 68  | GLU  | 7              |
| 1   | B     | 42  | SER  | 7              |
| 1   | B     | 25  | LYS  | 7              |
| 1   | B     | 4   | LEU  | 6              |
| 1   | A     | 2   | SER  | 6              |
| 1   | B     | 49  | LYS  | 6              |
| 1   | B     | 27  | LYS  | 6              |
| 1   | A     | 29  | SER  | 5              |
| 1   | A     | 85  | MET  | 4              |
| 1   | B     | 31  | LYS  | 4              |
| 1   | B     | 54  | VAL  | 4              |
| 1   | A     | 31  | LYS  | 4              |
| 1   | B     | 83  | VAL  | 4              |
| 1   | B     | 22  | GLU  | 4              |
| 1   | B     | 85  | MET  | 4              |
| 1   | B     | 87  | ASN  | 4              |
| 1   | A     | 34  | LYS  | 3              |
| 1   | A     | 39  | THR  | 3              |
| 1   | B     | 37  | LEU  | 3              |
| 1   | A     | 86  | ASN  | 3              |
| 1   | A     | 21  | LYS  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 87  | ASN  | 3              |
| 1   | A     | 16  | HIS  | 2              |
| 1   | A     | 8   | MET  | 2              |
| 1   | B     | 68  | GLU  | 2              |
| 1   | A     | 50  | ASP  | 2              |
| 1   | B     | 52  | ASP  | 2              |
| 1   | A     | 33  | LEU  | 1              |
| 1   | A     | 58  | MET  | 1              |
| 1   | B     | 64  | ASN  | 1              |
| 1   | A     | 64  | ASN  | 1              |
| 1   | A     | 89  | PHE  | 1              |
| 1   | B     | 35  | GLU  | 1              |
| 1   | A     | 40  | GLU  | 1              |
| 1   | B     | 9   | GLU  | 1              |
| 1   | B     | 21  | LYS  | 1              |
| 1   | B     | 33  | LEU  | 1              |
| 1   | A     | 49  | LYS  | 1              |
| 1   | B     | 58  | MET  | 1              |
| 1   | A     | 37  | LEU  | 1              |
| 1   | A     | 76  | VAL  | 1              |
| 1   | B     | 56  | LYS  | 1              |
| 1   | B     | 39  | THR  | 1              |
| 1   | A     | 52  | ASP  | 1              |
| 1   | A     | 44  | PHE  | 1              |
| 1   | A     | 56  | LYS  | 1              |
| 1   | B     | 8   | MET  | 1              |
| 1   | B     | 11  | LEU  | 1              |
| 1   | B     | 51  | VAL  | 1              |
| 1   | A     | 3   | GLU  | 1              |
| 1   | B     | 72  | GLN  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 46% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1148 |
| Number of shifts mapped to atoms        | 1148 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 93       | $-0.43 \pm 0.12$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 87       | $0.12 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 73       | $-0.36 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 86       | $0.45 \pm 0.22$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 47%, i.e. 1115 atoms were assigned a chemical shift out of a possible 2380. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 419/895 (47%)  | 177/364 (49%) | 159/354 (45%)   | 83/177 (47%)    |
| Sidechain | 619/1305 (47%) | 423/844 (50%) | 189/429 (44%)   | 7/32 (22%)      |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 77/180 (43%)    | 39/88 (44%)          | 37/83 (45%)           | 1/9 (11%)             |
| Overall  | 1115/2380 (47%) | 639/1296 (49%)       | 385/866 (44%)         | 91/218 (42%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 1148 atoms were assigned a chemical shift out of a possible 2476. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 437/942 (46%)   | 185/384 (48%)        | 166/372 (45%)         | 86/186 (46%)          |
| Sidechain | 634/1342 (47%)  | 433/866 (50%)        | 193/442 (44%)         | 8/34 (24%)            |
| Aromatic  | 77/192 (40%)    | 39/94 (41%)          | 37/88 (42%)           | 1/10 (10%)            |
| Overall   | 1148/2476 (46%) | 657/1344 (49%)       | 396/902 (44%)         | 95/230 (41%)          |

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

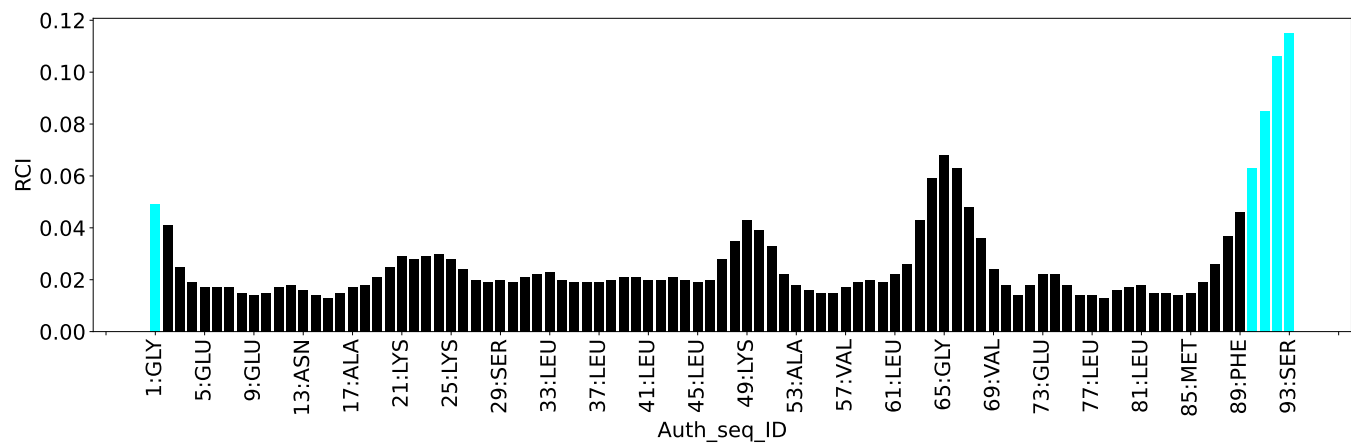
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 19  | SER  | HB3  | 2.42       | 2.49 – 5.20         | -5.3    |

#### 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                                | 3740  |
| Intra-residue ( $ i-j =0$ )                              | 756   |
| Sequential ( $ i-j =1$ )                                 | 986   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 1007  |
| Long range ( $ i-j \geq 5$ )                             | 645   |
| Inter-chain                                              | 346   |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 292   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 21.7  |
| Number of long range restraints per residue <sup>1</sup> | 3.5   |

<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)  | 64.5                                   | 0.2     |
| 0.2-0.5 (Medium) | 31.2                                   | 0.5     |
| >0.5 (Large)     | 43.8                                   | 4.08    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 3.5                                    | 4.77    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis

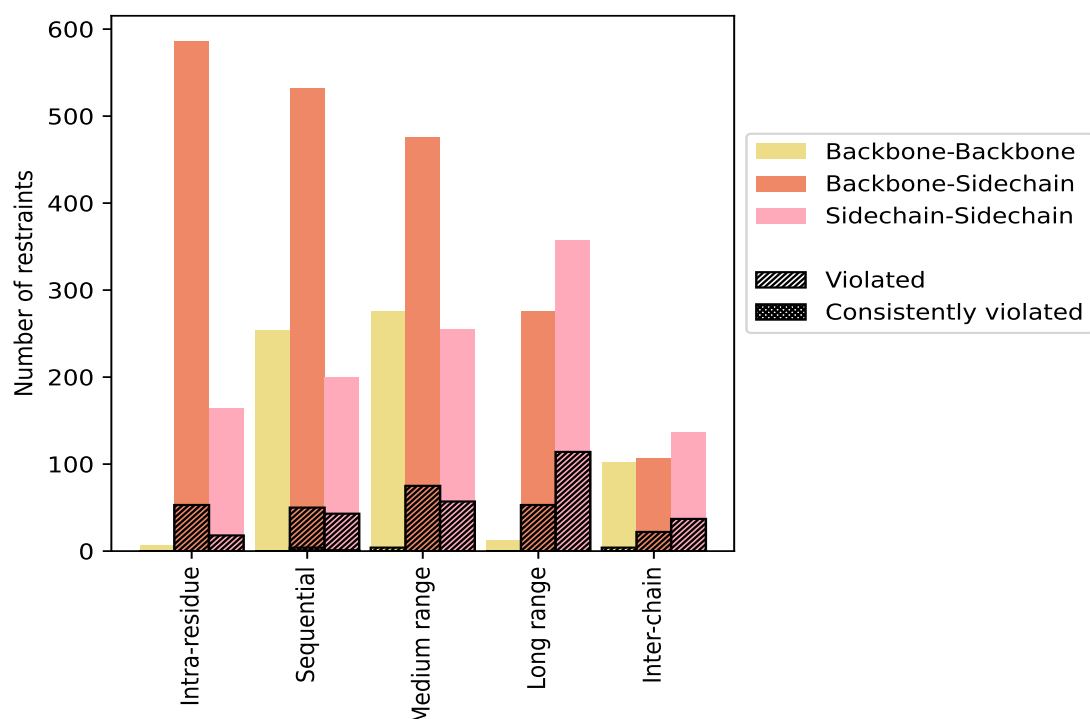
### 9.1 Summary of distance violations

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>756</b>  | <b>20.2</b>    | <b>71</b>             | <b>9.4</b>     | <b>1.9</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 6           | 0.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 586         | 15.7           | 53                    | 9.0            | 1.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 164         | 4.4            | 18                    | 11.0           | 0.5            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>986</b>  | <b>26.4</b>    | <b>93</b>             | <b>9.4</b>     | <b>2.5</b>     | <b>5</b>                           | <b>0.5</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 254         | 6.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 532         | 14.2           | 50                    | 9.4            | 1.3            | 4                                  | 0.8            | 0.1            |
| Sidechain-Sidechain                                                         | 200         | 5.3            | 43                    | 21.5           | 1.1            | 1                                  | 0.5            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>1007</b> | <b>26.9</b>    | <b>136</b>            | <b>13.5</b>    | <b>3.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 276         | 7.4            | 4                     | 1.4            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 476         | 12.7           | 75                    | 15.8           | 2.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 255         | 6.8            | 57                    | 22.4           | 1.5            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>645</b>  | <b>17.2</b>    | <b>167</b>            | <b>25.9</b>    | <b>4.5</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 12          | 0.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 276         | 7.4            | 53                    | 19.2           | 1.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 357         | 9.5            | 114                   | 31.9           | 3.0            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>346</b>  | <b>9.3</b>     | <b>63</b>             | <b>18.2</b>    | <b>1.7</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 102         | 2.7            | 4                     | 3.9            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 107         | 2.9            | 22                    | 20.6           | 0.6            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 137         | 3.7            | 37                    | 27.0           | 1.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>3740</b> | <b>100.0</b>   | <b>530</b>            | <b>14.2</b>    | <b>14.2</b>    | <b>5</b>                           | <b>0.1</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 650         | 17.4           | 8                     | 1.2            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1977        | 52.9           | 253                   | 12.8           | 6.8            | 4                                  | 0.2            | 0.1            |
| Sidechain-Sidechain                                                         | 1113        | 29.8           | 269                   | 24.2           | 7.2            | 1                                  | 0.1            | 0.0            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 19                   | 27              | 31              | 38              | 24              | 139   | 0.63     | 3.2     | 0.79                | 0.2        |
| 2        | 15                   | 33              | 35              | 52              | 25              | 160   | 0.75     | 3.26    | 0.87                | 0.24       |
| 3        | 22                   | 32              | 32              | 27              | 14              | 127   | 0.54     | 3.16    | 0.75                | 0.19       |
| 4        | 17                   | 23              | 38              | 39              | 19              | 136   | 0.5      | 3.07    | 0.69                | 0.2        |
| 5        | 18                   | 27              | 32              | 29              | 27              | 133   | 0.58     | 4.05    | 0.76                | 0.2        |
| 6        | 20                   | 27              | 35              | 39              | 13              | 134   | 0.47     | 2.61    | 0.65                | 0.18       |
| 7        | 21                   | 20              | 42              | 75              | 14              | 172   | 0.76     | 3.16    | 0.78                | 0.34       |
| 8        | 14                   | 30              | 32              | 40              | 25              | 141   | 0.63     | 3.38    | 0.81                | 0.2        |
| 9        | 22                   | 29              | 30              | 37              | 17              | 135   | 0.51     | 2.74    | 0.68                | 0.18       |
| 10       | 17                   | 31              | 39              | 35              | 21              | 143   | 0.61     | 3.01    | 0.79                | 0.19       |

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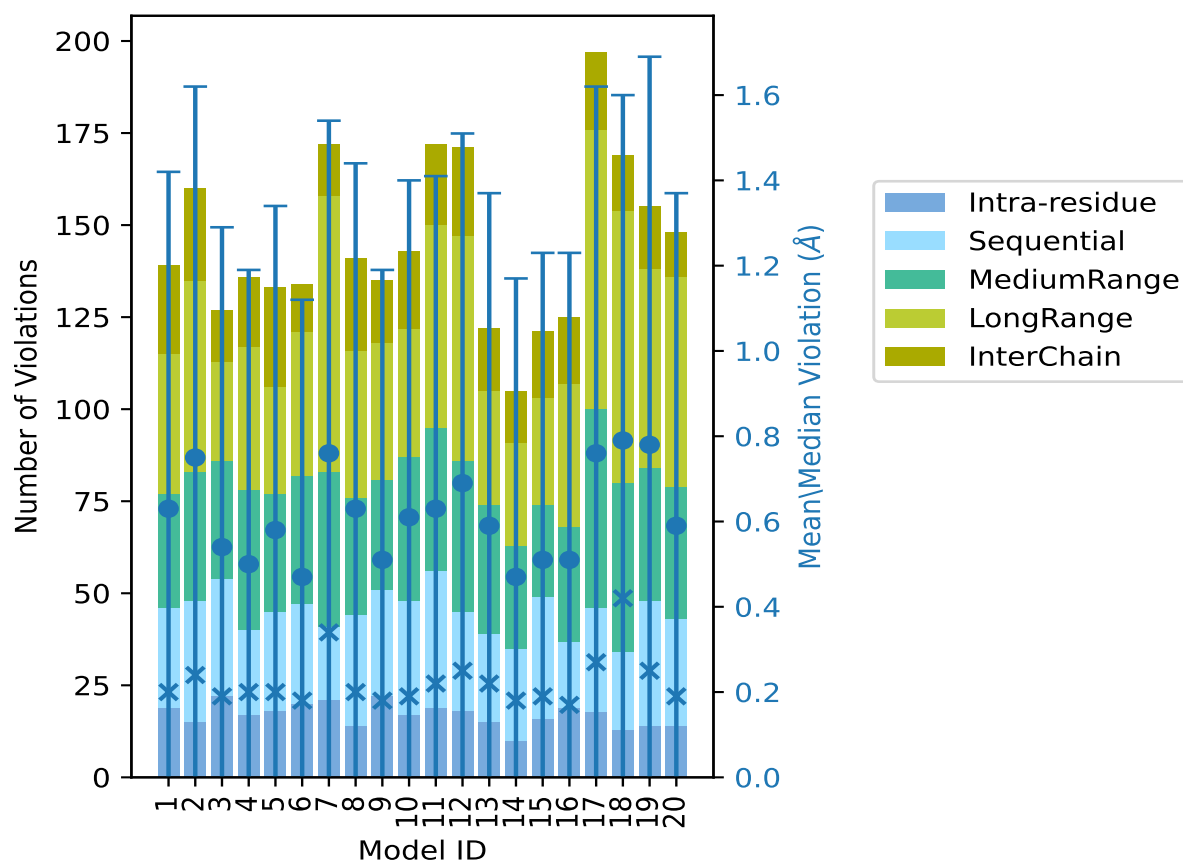
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 19                   | 37              | 39              | 55              | 22              | 172   | 0.63     | 3.53    | 0.78                | 0.22       |
| 12       | 18                   | 27              | 41              | 61              | 24              | 171   | 0.69     | 4.08    | 0.82                | 0.25       |
| 13       | 15                   | 24              | 35              | 31              | 17              | 122   | 0.59     | 2.8     | 0.78                | 0.22       |
| 14       | 10                   | 25              | 28              | 28              | 14              | 105   | 0.47     | 3.21    | 0.7                 | 0.18       |
| 15       | 16                   | 33              | 25              | 29              | 18              | 121   | 0.51     | 2.99    | 0.72                | 0.19       |
| 16       | 19                   | 18              | 31              | 39              | 18              | 125   | 0.51     | 3.01    | 0.72                | 0.17       |
| 17       | 18                   | 28              | 54              | 76              | 21              | 197   | 0.76     | 4.02    | 0.86                | 0.27       |
| 18       | 13                   | 21              | 46              | 74              | 15              | 169   | 0.79     | 3.72    | 0.81                | 0.42       |
| 19       | 14                   | 34              | 36              | 54              | 17              | 155   | 0.78     | 3.73    | 0.91                | 0.25       |
| 20       | 14                   | 29              | 36              | 57              | 12              | 148   | 0.59     | 4.02    | 0.78                | 0.19       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

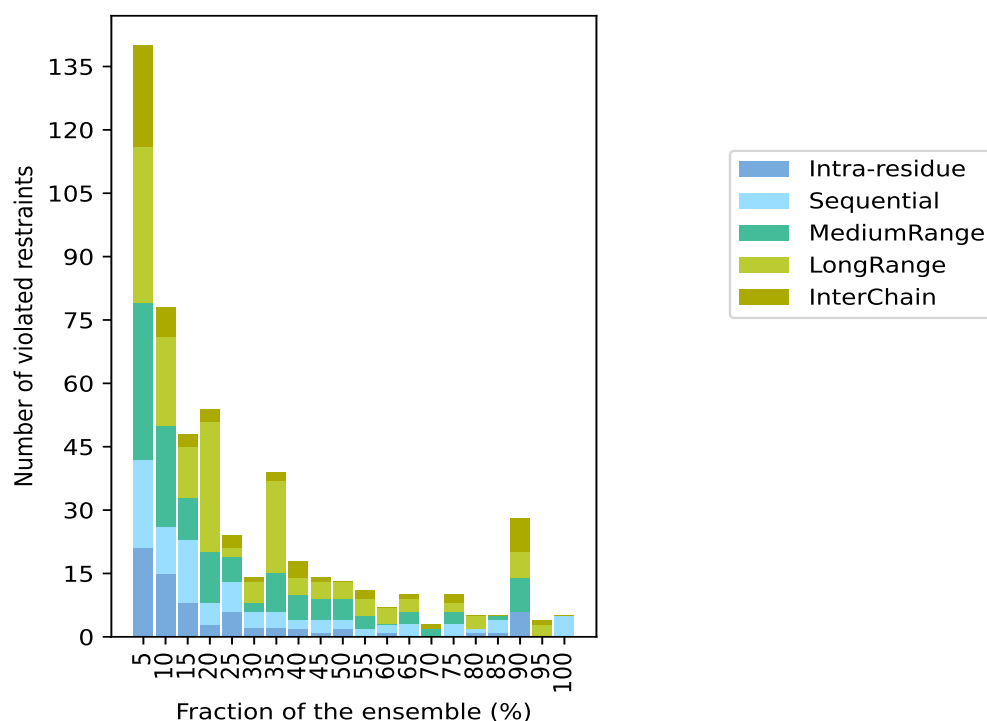
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3210(IR:685, SQ:893, MR:871, LR:478, IC:283) restraints are 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>       | %     |
| 21                            | 21              | 37              | 37              | 24              | 140   | 1                        | 5.0   |
| 15                            | 11              | 24              | 21              | 7               | 78    | 2                        | 10.0  |
| 8                             | 15              | 10              | 12              | 3               | 48    | 3                        | 15.0  |
| 3                             | 5               | 12              | 31              | 3               | 54    | 4                        | 20.0  |
| 6                             | 7               | 6               | 2               | 3               | 24    | 5                        | 25.0  |
| 2                             | 4               | 2               | 5               | 1               | 14    | 6                        | 30.0  |
| 2                             | 4               | 9               | 22              | 2               | 39    | 7                        | 35.0  |
| 2                             | 2               | 6               | 4               | 4               | 18    | 8                        | 40.0  |
| 1                             | 3               | 5               | 4               | 1               | 14    | 9                        | 45.0  |
| 2                             | 2               | 5               | 4               | 0               | 13    | 10                       | 50.0  |
| 0                             | 2               | 3               | 4               | 2               | 11    | 11                       | 55.0  |
| 1                             | 2               | 0               | 4               | 0               | 7     | 12                       | 60.0  |
| 0                             | 3               | 3               | 3               | 1               | 10    | 13                       | 65.0  |
| 0                             | 0               | 2               | 0               | 1               | 3     | 14                       | 70.0  |
| 0                             | 3               | 3               | 2               | 2               | 10    | 15                       | 75.0  |
| 1                             | 1               | 0               | 3               | 0               | 5     | 16                       | 80.0  |
| 1                             | 3               | 1               | 0               | 0               | 5     | 17                       | 85.0  |
| 6                             | 0               | 8               | 6               | 8               | 28    | 18                       | 90.0  |
| 0                             | 0               | 0               | 3               | 1               | 4     | 19                       | 95.0  |
| 0                             | 5               | 0               | 0               | 0               | 5     | 20                       | 100.0 |

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

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

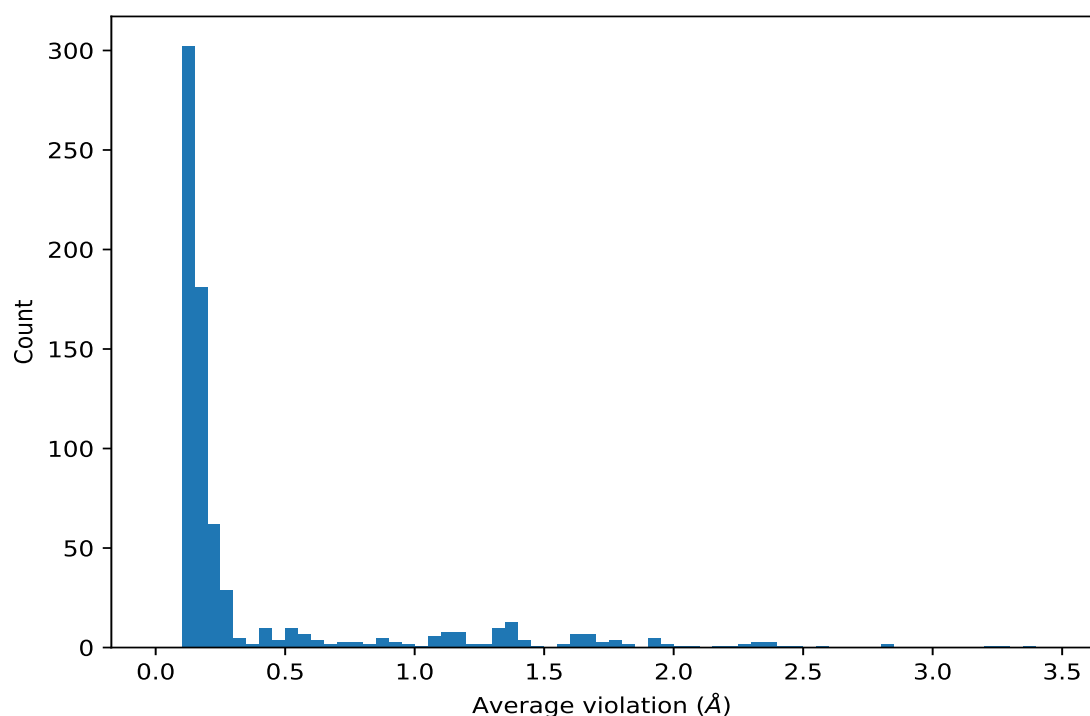
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG  | 20                  | 0.42     | 0.04                | 0.42       |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2 | 20                  | 0.25     | 0.08                | 0.24       |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2 | 20                  | 0.25     | 0.08                | 0.24       |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2 | 20                  | 0.25     | 0.08                | 0.24       |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG  | 20                  | 0.24     | 0.07                | 0.22       |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H   | 20                  | 0.17     | 0.04                | 0.17       |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H   | 20                  | 0.17     | 0.04                | 0.17       |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H   | 20                  | 0.17     | 0.04                | 0.17       |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H   | 20                  | 0.17     | 0.03                | 0.17       |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H   | 20                  | 0.17     | 0.03                | 0.17       |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H   | 20                  | 0.17     | 0.03                | 0.17       |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1 | 19                  | 1.36     | 0.49                | 1.39       |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1 | 19                  | 1.36     | 0.49                | 1.39       |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1 | 19                  | 1.36     | 0.49                | 1.39       |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1 | 19                  | 1.16     | 0.59                | 1.09       |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1 | 19                  | 1.16     | 0.59                | 1.09       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 19                  | 1.16     | 0.59                | 1.09       |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 19                  | 0.15     | 0.03                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,887)  | 1:44:A:PHE:HE2  | 1:85:A:MET:HB2  | 18                  | 2.58     | 0.49                | 2.76       |
| (1,46)   | 1:8:A:MET:H     | 1:44:B:PHE:HE1  | 18                  | 2.49     | 0.37                | 2.46       |
| (1,188)  | 1:44:A:PHE:HE1  | 1:8:B:MET:H     | 18                  | 2.44     | 0.32                | 2.49       |
| (1,1421) | 1:41:A:LEU:HA   | 1:44:A:PHE:HD1  | 18                  | 2.4      | 0.14                | 2.38       |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG2  | 18                  | 2.38     | 0.47                | 2.46       |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG3  | 18                  | 2.38     | 0.47                | 2.46       |
| (1,29)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HD1  | 18                  | 2.34     | 0.27                | 2.37       |
| (1,197)  | 1:44:A:PHE:HD1  | 1:5:B:GLU:HA    | 18                  | 2.34     | 0.18                | 2.38       |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2  | 18                  | 2.33     | 0.6                 | 2.5        |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG2  | 18                  | 2.26     | 0.46                | 2.32       |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG3  | 18                  | 2.26     | 0.46                | 2.32       |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1  | 18                  | 2.24     | 0.24                | 2.24       |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 18                  | 1.99     | 0.16                | 1.94       |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 18                  | 1.99     | 0.5                 | 2.13       |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 18                  | 1.94     | 0.34                | 1.91       |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 18                  | 1.92     | 0.31                | 1.91       |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 18                  | 1.6      | 0.32                | 1.72       |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 18                  | 1.41     | 0.35                | 1.35       |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 18                  | 1.23     | 0.17                | 1.23       |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 18                  | 1.12     | 0.23                | 1.14       |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 18                  | 1.06     | 0.27                | 1.17       |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 18                  | 1.06     | 0.27                | 1.17       |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 18                  | 1.06     | 0.27                | 1.17       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 18                  | 0.86     | 0.32                | 0.84       |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 18                  | 0.86     | 0.32                | 0.84       |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 18                  | 0.86     | 0.32                | 0.84       |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 18                  | 0.69     | 0.18                | 0.74       |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 18                  | 0.6      | 0.27                | 0.57       |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 18                  | 0.23     | 0.03                | 0.24       |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 18                  | 0.22     | 0.05                | 0.22       |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 18                  | 0.22     | 0.05                | 0.22       |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 18                  | 0.22     | 0.05                | 0.22       |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 18                  | 0.21     | 0.04                | 0.21       |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,334)  | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,334)  | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 18                  | 0.14     | 0.03                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,329)  | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 18                  | 0.13     | 0.02                | 0.13       |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 17                  | 0.28     | 0.07                | 0.27       |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 17                  | 0.21     | 0.05                | 0.22       |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 17                  | 0.21     | 0.05                | 0.22       |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 17                  | 0.21     | 0.05                | 0.22       |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 17                  | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 17                  | 0.18     | 0.05                | 0.2        |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 17                  | 0.17     | 0.05                | 0.16       |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1  | 16                  | 1.78     | 1.2                 | 2.24       |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2  | 16                  | 1.78     | 1.2                 | 2.24       |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3  | 16                  | 1.78     | 1.2                 | 2.24       |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 16                  | 1.7      | 1.09                | 1.92       |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 16                  | 1.7      | 1.09                | 1.92       |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 16                  | 1.7      | 1.09                | 1.92       |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 16                  | 0.54     | 0.31                | 0.52       |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 16                  | 0.21     | 0.06                | 0.22       |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 16                  | 0.16     | 0.03                | 0.16       |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 15                  | 0.28     | 0.09                | 0.32       |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 15                  | 0.25     | 0.05                | 0.26       |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 15                  | 0.21     | 0.05                | 0.2        |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 15                  | 0.19     | 0.06                | 0.15       |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 15                  | 0.18     | 0.05                | 0.16       |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 15                  | 0.18     | 0.05                | 0.16       |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 15                  | 0.18     | 0.05                | 0.16       |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 15                  | 0.16     | 0.04                | 0.17       |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 15                  | 0.16     | 0.04                | 0.16       |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 15                  | 0.16     | 0.04                | 0.16       |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 15                  | 0.16     | 0.04                | 0.16       |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 15                  | 0.15     | 0.03                | 0.15       |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 15                  | 0.15     | 0.03                | 0.15       |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 15                  | 0.15     | 0.03                | 0.15       |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 15                  | 0.15     | 0.03                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 15                  | 0.15     | 0.03                | 0.14       |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 15                  | 0.15     | 0.03                | 0.14       |
| (1,956)  | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 15                  | 0.15     | 0.03                | 0.14       |
| (1,956)  | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 15                  | 0.15     | 0.03                | 0.14       |
| (1,956)  | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 15                  | 0.15     | 0.03                | 0.14       |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 14                  | 0.17     | 0.03                | 0.16       |
| (1,165)  | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 14                  | 0.16     | 0.06                | 0.14       |
| (1,165)  | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 14                  | 0.16     | 0.06                | 0.14       |
| (1,165)  | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 14                  | 0.16     | 0.06                | 0.14       |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 14                  | 0.13     | 0.02                | 0.13       |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 14                  | 0.13     | 0.02                | 0.13       |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 14                  | 0.13     | 0.02                | 0.13       |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1  | 13                  | 1.91     | 1.04                | 2.25       |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2  | 13                  | 1.91     | 1.04                | 2.25       |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3  | 13                  | 1.91     | 1.04                | 2.25       |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1  | 13                  | 1.61     | 0.96                | 1.45       |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2  | 13                  | 1.61     | 0.96                | 1.45       |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3  | 13                  | 1.61     | 0.96                | 1.45       |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 13                  | 0.5      | 0.27                | 0.46       |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 13                  | 0.2      | 0.1                 | 0.18       |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 13                  | 0.19     | 0.07                | 0.17       |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 13                  | 0.18     | 0.05                | 0.18       |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 13                  | 0.18     | 0.05                | 0.16       |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 13                  | 0.18     | 0.05                | 0.16       |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 13                  | 0.18     | 0.05                | 0.16       |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 13                  | 0.17     | 0.04                | 0.16       |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 13                  | 0.17     | 0.04                | 0.16       |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 13                  | 0.17     | 0.04                | 0.16       |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 13                  | 0.14     | 0.03                | 0.13       |
| (1,176)  | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 13                  | 0.14     | 0.04                | 0.13       |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 12                  | 1.66     | 1.13                | 1.42       |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 12                  | 0.39     | 0.2                 | 0.28       |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 12                  | 0.2      | 0.08                | 0.16       |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 12                  | 0.19     | 0.06                | 0.18       |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 12                  | 0.17     | 0.04                | 0.17       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 12                  | 0.17     | 0.04                | 0.17       |
| (1,276)  | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,967)  | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 12                  | 0.15     | 0.04                | 0.13       |
| (1,967)  | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 12                  | 0.15     | 0.04                | 0.13       |
| (1,967)  | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 12                  | 0.15     | 0.04                | 0.13       |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 11                  | 1.43     | 0.87                | 1.59       |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 11                  | 0.87     | 0.15                | 0.92       |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 11                  | 0.87     | 0.15                | 0.92       |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 11                  | 0.27     | 0.11                | 0.28       |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 11                  | 0.2      | 0.08                | 0.15       |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 11                  | 0.2      | 0.08                | 0.15       |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 11                  | 0.2      | 0.08                | 0.15       |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 11                  | 0.18     | 0.04                | 0.16       |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 11                  | 0.17     | 0.05                | 0.15       |
| (1,399)  | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 11                  | 0.16     | 0.03                | 0.18       |
| (1,437)  | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 11                  | 0.15     | 0.04                | 0.15       |
| (1,437)  | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 11                  | 0.15     | 0.04                | 0.15       |
| (1,437)  | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 11                  | 0.15     | 0.04                | 0.15       |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 11                  | 0.14     | 0.02                | 0.14       |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 11                  | 0.14     | 0.03                | 0.12       |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 11                  | 0.13     | 0.03                | 0.13       |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 10                  | 0.99     | 0.86                | 0.56       |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1  | 10                  | 0.81     | 0.26                | 0.86       |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 10                  | 0.71     | 0.16                | 0.74       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 10                  | 0.71     | 0.16                | 0.74       |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 10                  | 0.28     | 0.11                | 0.28       |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 10                  | 0.23     | 0.09                | 0.2        |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 10                  | 0.22     | 0.07                | 0.2        |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 10                  | 0.21     | 0.08                | 0.2        |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 10                  | 0.21     | 0.1                 | 0.15       |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 10                  | 0.2      | 0.03                | 0.2        |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 10                  | 0.2      | 0.03                | 0.2        |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 10                  | 0.2      | 0.03                | 0.2        |
| (1,395)  | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 10                  | 0.18     | 0.05                | 0.18       |
| (1,429)  | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 10                  | 0.18     | 0.02                | 0.17       |
| (1,267)  | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2  | 10                  | 0.15     | 0.03                | 0.14       |
| (1,267)  | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2  | 10                  | 0.15     | 0.03                | 0.14       |
| (1,267)  | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2  | 10                  | 0.15     | 0.03                | 0.14       |
| (1,289)  | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 10                  | 0.12     | 0.02                | 0.12       |
| (1,289)  | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 10                  | 0.12     | 0.02                | 0.12       |
| (1,289)  | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 10                  | 0.12     | 0.02                | 0.12       |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 9                   | 1.14     | 0.4                 | 1.25       |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 9                   | 0.52     | 0.18                | 0.45       |
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 9                   | 0.26     | 0.06                | 0.28       |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 9                   | 0.26     | 0.1                 | 0.24       |
| (1,2472) | 1:59:A:LYS:HG3  | 1:60:A:GLU:HB2  | 9                   | 0.24     | 0.12                | 0.17       |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 9                   | 0.18     | 0.08                | 0.17       |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 9                   | 0.17     | 0.04                | 0.16       |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 9                   | 0.17     | 0.04                | 0.17       |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 9                   | 0.17     | 0.04                | 0.16       |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 9                   | 0.17     | 0.04                | 0.16       |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 9                   | 0.17     | 0.04                | 0.16       |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 9                   | 0.16     | 0.05                | 0.15       |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 9                   | 0.16     | 0.04                | 0.16       |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 9                   | 0.16     | 0.04                | 0.16       |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 9                   | 0.16     | 0.04                | 0.16       |
| (1,963)  | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 9                   | 0.15     | 0.05                | 0.13       |
| (1,535)  | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 9                   | 0.14     | 0.02                | 0.14       |
| (1,535)  | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 9                   | 0.14     | 0.02                | 0.14       |
| (1,535)  | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 9                   | 0.14     | 0.02                | 0.14       |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 9                   | 0.13     | 0.03                | 0.12       |
| (1,205)  | 1:90:A:TRP:HA   | 1:26:B:TYR:HE1  | 8                   | 3.23     | 0.4                 | 3.14       |
| (1,204)  | 1:90:A:TRP:HB3  | 1:26:B:TYR:HE1  | 8                   | 2.07     | 0.49                | 1.96       |
| (1,1016) | 1:16:B:HIS:HE1  | 1:26:B:TYR:HD1  | 8                   | 1.65     | 1.42                | 1.12       |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 8                   | 1.58     | 0.35                | 1.52       |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 8                   | 1.39     | 0.35                | 1.4        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2  | 8                   | 0.43     | 0.04                | 0.42       |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 8                   | 0.29     | 0.08                | 0.29       |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2  | 8                   | 0.27     | 0.11                | 0.27       |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 8                   | 0.22     | 0.05                | 0.22       |
| (1,522)  | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 8                   | 0.21     | 0.08                | 0.18       |
| (1,522)  | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 8                   | 0.21     | 0.08                | 0.18       |
| (1,538)  | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 8                   | 0.19     | 0.08                | 0.15       |
| (1,538)  | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 8                   | 0.19     | 0.08                | 0.15       |
| (1,538)  | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 8                   | 0.19     | 0.08                | 0.15       |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,566)  | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 8                   | 0.17     | 0.04                | 0.17       |
| (1,566)  | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 8                   | 0.17     | 0.04                | 0.17       |
| (1,566)  | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 8                   | 0.17     | 0.04                | 0.17       |
| (1,559)  | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 8                   | 0.17     | 0.04                | 0.16       |
| (1,559)  | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 8                   | 0.17     | 0.04                | 0.16       |
| (1,559)  | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 8                   | 0.17     | 0.04                | 0.16       |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 8                   | 0.17     | 0.04                | 0.17       |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 8                   | 0.17     | 0.04                | 0.17       |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 8                   | 0.17     | 0.04                | 0.17       |
| (1,575)  | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 8                   | 0.14     | 0.03                | 0.15       |
| (1,575)  | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 8                   | 0.14     | 0.03                | 0.15       |
| (1,575)  | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 8                   | 0.14     | 0.03                | 0.15       |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 8                   | 0.14     | 0.03                | 0.12       |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 8                   | 0.14     | 0.03                | 0.12       |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 8                   | 0.14     | 0.03                | 0.12       |
| (1,286)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 8                   | 0.12     | 0.01                | 0.13       |
| (1,286)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 8                   | 0.12     | 0.01                | 0.13       |
| (1,286)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 8                   | 0.12     | 0.01                | 0.13       |
| (1,3540) | 1:15:B:PHE:HE2  | 1:26:B:TYR:H    | 7                   | 3.36     | 0.32                | 3.26       |
| (1,2788) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HA   | 7                   | 2.81     | 0.19                | 2.76       |
| (1,2312) | 1:15:B:PHE:HD2  | 1:26:B:TYR:HA   | 7                   | 2.15     | 0.26                | 2.26       |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3  | 7                   | 1.8      | 0.29                | 1.68       |
| (1,2685) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB2  | 7                   | 1.75     | 0.41                | 1.83       |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 7                   | 1.73     | 0.35                | 1.92       |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD12 | 7                   | 1.73     | 0.35                | 1.92       |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD13 | 7                   | 1.73     | 0.35                | 1.92       |
| (1,1901) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB2  | 7                   | 1.62     | 0.37                | 1.58       |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA   | 7                   | 1.56     | 0.34                | 1.6        |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 7                   | 1.42     | 0.35                | 1.52       |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3  | 7                   | 1.38     | 0.34                | 1.29       |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 7                   | 1.35     | 0.37                | 1.12       |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 7                   | 1.35     | 0.37                | 1.12       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2589) | 1:15:B:PHE:HD1 | 1:69:B:VAL:HG13 | 7                   | 1.35     | 0.37                | 1.12       |
| (1,882)  | 1:15:B:PHE:HD1 | 1:74:B:TYR:HD2  | 7                   | 1.33     | 0.08                | 1.31       |
| (1,1966) | 1:15:B:PHE:HD1 | 1:69:B:VAL:HG21 | 7                   | 1.31     | 0.15                | 1.35       |
| (1,1966) | 1:15:B:PHE:HD1 | 1:69:B:VAL:HG22 | 7                   | 1.31     | 0.15                | 1.35       |
| (1,1966) | 1:15:B:PHE:HD1 | 1:69:B:VAL:HG23 | 7                   | 1.31     | 0.15                | 1.35       |
| (1,1676) | 1:15:B:PHE:HE1 | 1:28:B:LEU:HD21 | 7                   | 1.17     | 0.2                 | 1.17       |
| (1,1676) | 1:15:B:PHE:HE1 | 1:28:B:LEU:HD22 | 7                   | 1.17     | 0.2                 | 1.17       |
| (1,1676) | 1:15:B:PHE:HE1 | 1:28:B:LEU:HD23 | 7                   | 1.17     | 0.2                 | 1.17       |
| (1,3541) | 1:15:B:PHE:HD2 | 1:19:B:SER:HA   | 7                   | 1.16     | 0.38                | 0.99       |
| (1,3274) | 1:15:B:PHE:HE2 | 1:27:B:LYS:HB2  | 7                   | 1.11     | 0.23                | 1.03       |
| (1,2724) | 1:15:B:PHE:HE1 | 1:28:B:LEU:HG   | 7                   | 1.1      | 0.26                | 1.18       |
| (1,1058) | 1:15:B:PHE:HD1 | 1:28:B:LEU:HD21 | 7                   | 1.07     | 0.28                | 0.93       |
| (1,1058) | 1:15:B:PHE:HD1 | 1:28:B:LEU:HD22 | 7                   | 1.07     | 0.28                | 0.93       |
| (1,1058) | 1:15:B:PHE:HD1 | 1:28:B:LEU:HD23 | 7                   | 1.07     | 0.28                | 0.93       |
| (1,2294) | 1:15:B:PHE:HE1 | 1:74:B:TYR:HD2  | 7                   | 0.94     | 0.07                | 0.94       |
| (1,1810) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HE2  | 7                   | 0.79     | 0.1                 | 0.84       |
| (1,2949) | 1:15:B:PHE:HE2 | 1:19:B:SER:HA   | 7                   | 0.75     | 0.39                | 0.63       |
| (1,210)  | 1:91:A:GLU:HG3 | 1:26:B:TYR:HE1  | 7                   | 0.63     | 0.55                | 0.42       |
| (1,2528) | 1:15:B:PHE:HE1 | 1:74:B:TYR:HB3  | 7                   | 0.56     | 0.13                | 0.56       |
| (1,1695) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG21 | 7                   | 0.54     | 0.07                | 0.55       |
| (1,1695) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG22 | 7                   | 0.54     | 0.07                | 0.55       |
| (1,1695) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG23 | 7                   | 0.54     | 0.07                | 0.55       |
| (1,203)  | 1:90:A:TRP:HB2 | 1:26:B:TYR:HE1  | 7                   | 0.51     | 0.36                | 0.32       |
| (1,2080) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD21 | 7                   | 0.45     | 0.19                | 0.52       |
| (1,2080) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD22 | 7                   | 0.45     | 0.19                | 0.52       |
| (1,2080) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD23 | 7                   | 0.45     | 0.19                | 0.52       |
| (1,1952) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG11 | 7                   | 0.44     | 0.31                | 0.28       |
| (1,1952) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG12 | 7                   | 0.44     | 0.31                | 0.28       |
| (1,1952) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG13 | 7                   | 0.44     | 0.31                | 0.28       |
| (1,3484) | 1:57:A:VAL:H   | 1:58:A:MET:HG2  | 7                   | 0.42     | 0.04                | 0.43       |
| (1,2329) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HB3  | 7                   | 0.31     | 0.15                | 0.26       |
| (1,3615) | 1:58:B:MET:HG2 | 1:59:B:LYS:HB2  | 7                   | 0.26     | 0.06                | 0.25       |
| (1,1616) | 1:30:A:LYS:HE2 | 1:33:A:LEU:HB3  | 7                   | 0.23     | 0.12                | 0.16       |
| (1,524)  | 1:59:B:LYS:HB2 | 1:59:B:LYS:HE2  | 7                   | 0.23     | 0.11                | 0.19       |
| (1,524)  | 1:59:B:LYS:HB2 | 1:59:B:LYS:HE3  | 7                   | 0.23     | 0.11                | 0.19       |
| (1,3275) | 1:26:A:TYR:HA  | 1:27:A:LYS:HD2  | 7                   | 0.21     | 0.06                | 0.22       |
| (1,3489) | 1:63:A:GLU:HA  | 1:66:A:ASP:HB2  | 7                   | 0.19     | 0.06                | 0.21       |
| (1,390)  | 1:30:B:LYS:HG3 | 1:65:B:GLY:HA3  | 7                   | 0.18     | 0.03                | 0.19       |
| (1,1593) | 1:25:B:LYS:HB2 | 1:25:B:LYS:HE3  | 7                   | 0.15     | 0.04                | 0.14       |
| (1,726)  | 1:18:A:HIS:HB3 | 1:28:A:LEU:HD11 | 7                   | 0.15     | 0.04                | 0.13       |
| (1,726)  | 1:18:A:HIS:HB3 | 1:28:A:LEU:HD12 | 7                   | 0.15     | 0.04                | 0.13       |
| (1,726)  | 1:18:A:HIS:HB3 | 1:28:A:LEU:HD13 | 7                   | 0.15     | 0.04                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2364) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG2  | 7                   | 0.14     | 0.02                | 0.13       |
| (1,572)  | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,572)  | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,572)  | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,3105) | 1:15:B:PHE:HE1  | 1:70:B:ASP:HB3  | 6                   | 0.53     | 0.26                | 0.55       |
| (1,2205) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB2  | 6                   | 0.48     | 0.16                | 0.42       |
| (1,3550) | 1:22:B:GLU:HB2  | 1:29:B:SER:HA   | 6                   | 0.22     | 0.06                | 0.2        |
| (1,3470) | 1:48:A:GLN:HE22 | 1:49:A:LYS:H    | 6                   | 0.2      | 0.07                | 0.2        |
| (1,3279) | 1:26:B:TYR:HA   | 1:27:B:LYS:HD2  | 6                   | 0.2      | 0.06                | 0.22       |
| (1,1395) | 1:31:B:LYS:HB2  | 1:32:B:GLU:H    | 6                   | 0.19     | 0.06                | 0.2        |
| (1,39)   | 1:4:A:LEU:HD21  | 1:40:B:GLU:HA   | 6                   | 0.18     | 0.11                | 0.12       |
| (1,39)   | 1:4:A:LEU:HD22  | 1:40:B:GLU:HA   | 6                   | 0.18     | 0.11                | 0.12       |
| (1,39)   | 1:4:A:LEU:HD23  | 1:40:B:GLU:HA   | 6                   | 0.18     | 0.11                | 0.12       |
| (1,2563) | 1:31:A:LYS:HG3  | 1:32:A:GLU:HG3  | 6                   | 0.17     | 0.04                | 0.16       |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD21  | 6                   | 0.16     | 0.06                | 0.14       |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD22  | 6                   | 0.16     | 0.06                | 0.14       |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD23  | 6                   | 0.16     | 0.06                | 0.14       |
| (1,387)  | 1:60:A:GLU:HA   | 1:60:A:GLU:HG3  | 6                   | 0.15     | 0.01                | 0.16       |
| (1,3400) | 1:9:A:GLU:HA    | 1:71:A:PHE:HE2  | 6                   | 0.14     | 0.04                | 0.14       |
| (1,314)  | 1:56:B:LYS:HB2  | 1:56:B:LYS:HD2  | 6                   | 0.14     | 0.03                | 0.14       |
| (1,3575) | 1:37:B:LEU:HB2  | 1:74:B:TYR:HA   | 6                   | 0.13     | 0.02                | 0.14       |
| (1,412)  | 1:72:B:GLN:HA   | 1:75:B:VAL:HG21 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,412)  | 1:72:B:GLN:HA   | 1:75:B:VAL:HG22 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,412)  | 1:72:B:GLN:HA   | 1:75:B:VAL:HG23 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,3413) | 1:15:A:PHE:HD2  | 1:19:A:SER:HA   | 5                   | 1.1      | 0.54                | 1.26       |
| (1,946)  | 1:25:B:LYS:HB2  | 1:26:B:TYR:HD1  | 5                   | 0.95     | 0.33                | 1.08       |
| (1,254)  | 1:89:A:PHE:HD2  | 1:9:B:GLU:HG2   | 5                   | 0.85     | 0.53                | 1.15       |
| (1,2331) | 1:25:B:LYS:HA   | 1:26:B:TYR:HD1  | 5                   | 0.76     | 0.21                | 0.88       |
| (1,3516) | 1:89:A:PHE:H    | 1:89:A:PHE:HE2  | 5                   | 0.42     | 0.17                | 0.34       |
| (1,2107) | 1:25:B:LYS:HG3  | 1:26:B:TYR:HA   | 5                   | 0.28     | 0.04                | 0.27       |
| (1,2991) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HA   | 5                   | 0.26     | 0.04                | 0.25       |
| (1,2987) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HA   | 5                   | 0.25     | 0.06                | 0.26       |
| (1,3476) | 1:51:A:VAL:H    | 1:55:A:ASP:H    | 5                   | 0.23     | 0.02                | 0.23       |
| (1,927)  | 1:21:B:LYS:HA   | 1:21:B:LYS:HE2  | 5                   | 0.22     | 0.07                | 0.25       |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD11  | 5                   | 0.19     | 0.02                | 0.18       |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD12  | 5                   | 0.19     | 0.02                | 0.18       |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD13  | 5                   | 0.19     | 0.02                | 0.18       |
| (1,2103) | 1:63:A:GLU:HB2  | 1:64:A:ASN:HD21 | 5                   | 0.19     | 0.07                | 0.2        |
| (1,3385) | 1:66:A:ASP:HB2  | 1:68:A:GLU:H    | 5                   | 0.17     | 0.05                | 0.17       |
| (1,918)  | 1:31:A:LYS:H    | 1:31:A:LYS:HG2  | 5                   | 0.16     | 0.02                | 0.15       |
| (1,339)  | 1:12:A:ILE:HG21 | 1:16:A:HIS:HD2  | 5                   | 0.16     | 0.04                | 0.14       |
| (1,339)  | 1:12:A:ILE:HG22 | 1:16:A:HIS:HD2  | 5                   | 0.16     | 0.04                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,339)  | 1:12:A:ILE:HG23 | 1:16:A:HIS:HD2  | 5                   | 0.16     | 0.04                | 0.14       |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD21  | 5                   | 0.16     | 0.06                | 0.13       |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD22  | 5                   | 0.16     | 0.06                | 0.13       |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD23  | 5                   | 0.16     | 0.06                | 0.13       |
| (1,81)   | 1:72:A:GLN:HA   | 1:80:B:ALA:HA   | 5                   | 0.15     | 0.04                | 0.14       |
| (1,2370) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG2  | 5                   | 0.14     | 0.03                | 0.14       |
| (1,3533) | 1:14:B:VAL:HA   | 1:74:B:TYR:HE2  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,952)  | 1:29:A:SER:HB3  | 1:68:A:GLU:HG3  | 5                   | 0.14     | 0.01                | 0.14       |
| (1,539)  | 1:80:B:ALA:HA   | 1:83:B:VAL:HG11 | 5                   | 0.13     | 0.03                | 0.13       |
| (1,539)  | 1:80:B:ALA:HA   | 1:83:B:VAL:HG12 | 5                   | 0.13     | 0.03                | 0.13       |
| (1,539)  | 1:80:B:ALA:HA   | 1:83:B:VAL:HG13 | 5                   | 0.13     | 0.03                | 0.13       |
| (1,259)  | 1:37:A:LEU:HD21 | 1:41:A:LEU:HB2  | 5                   | 0.13     | 0.03                | 0.11       |
| (1,259)  | 1:37:A:LEU:HD22 | 1:41:A:LEU:HB2  | 5                   | 0.13     | 0.03                | 0.11       |
| (1,259)  | 1:37:A:LEU:HD23 | 1:41:A:LEU:HB2  | 5                   | 0.13     | 0.03                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,75)   | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,739)  | 1:12:A:ILE:HA   | 1:12:A:ILE:HD11 | 5                   | 0.11     | 0.01                | 0.1        |
| (1,739)  | 1:12:A:ILE:HA   | 1:12:A:ILE:HD12 | 5                   | 0.11     | 0.01                | 0.1        |
| (1,739)  | 1:12:A:ILE:HA   | 1:12:A:ILE:HD13 | 5                   | 0.11     | 0.01                | 0.1        |
| (1,3412) | 1:15:A:PHE:HE2  | 1:26:A:TYR:H    | 4                   | 3.28     | 0.35                | 3.3        |
| (1,2780) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HA   | 4                   | 2.82     | 0.15                | 2.84       |
| (1,2307) | 1:15:A:PHE:HD2  | 1:26:A:TYR:HA   | 4                   | 2.05     | 0.37                | 2.13       |
| (1,2251) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB3  | 4                   | 1.8      | 0.2                 | 1.76       |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD11 | 4                   | 1.68     | 0.32                | 1.73       |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD12 | 4                   | 1.68     | 0.32                | 1.73       |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD13 | 4                   | 1.68     | 0.32                | 1.73       |
| (1,2676) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB2  | 4                   | 1.61     | 0.24                | 1.63       |
| (1,1897) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB2  | 4                   | 1.49     | 0.26                | 1.52       |
| (1,2910) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HG2  | 4                   | 1.43     | 0.22                | 1.39       |
| (1,2086) | 1:15:A:PHE:HE2  | 1:26:A:TYR:HA   | 4                   | 1.4      | 0.35                | 1.5        |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG11 | 4                   | 1.37     | 0.25                | 1.25       |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG12 | 4                   | 1.37     | 0.25                | 1.25       |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG13 | 4                   | 1.37     | 0.25                | 1.25       |
| (1,1992) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB3  | 4                   | 1.36     | 0.2                 | 1.32       |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG21 | 4                   | 1.33     | 0.14                | 1.36       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG22 | 4                   | 1.33     | 0.14                | 1.36       |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG23 | 4                   | 1.33     | 0.14                | 1.36       |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD21 | 4                   | 1.32     | 0.26                | 1.34       |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD22 | 4                   | 1.32     | 0.26                | 1.34       |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD23 | 4                   | 1.32     | 0.26                | 1.34       |
| (1,876)  | 1:15:A:PHE:HD1  | 1:74:A:TYR:HD2  | 4                   | 1.28     | 0.17                | 1.19       |
| (1,2710) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HG   | 4                   | 1.26     | 0.31                | 1.23       |
| (1,3125) | 1:86:A:ASN:HB3  | 1:89:A:PHE:HD2  | 4                   | 1.21     | 0.77                | 1.34       |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD21 | 4                   | 1.14     | 0.23                | 1.16       |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD22 | 4                   | 1.14     | 0.23                | 1.16       |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD23 | 4                   | 1.14     | 0.23                | 1.16       |
| (1,3272) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HB2  | 4                   | 1.01     | 0.25                | 0.92       |
| (1,2938) | 1:15:A:PHE:HE2  | 1:19:A:SER:HA   | 4                   | 0.96     | 0.21                | 0.92       |
| (1,2287) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HD2  | 4                   | 0.94     | 0.13                | 0.9        |
| (1,1800) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HE2  | 4                   | 0.72     | 0.1                 | 0.75       |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG21 | 4                   | 0.63     | 0.1                 | 0.65       |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG22 | 4                   | 0.63     | 0.1                 | 0.65       |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG23 | 4                   | 0.63     | 0.1                 | 0.65       |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG11 | 4                   | 0.56     | 0.32                | 0.46       |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG12 | 4                   | 0.56     | 0.32                | 0.46       |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG13 | 4                   | 0.56     | 0.32                | 0.46       |
| (1,2522) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB3  | 4                   | 0.55     | 0.26                | 0.64       |
| (1,2198) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB2  | 4                   | 0.53     | 0.19                | 0.61       |
| (1,3101) | 1:15:A:PHE:HE1  | 1:70:A:ASP:HB3  | 4                   | 0.51     | 0.14                | 0.58       |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD21 | 4                   | 0.43     | 0.08                | 0.42       |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD22 | 4                   | 0.43     | 0.08                | 0.42       |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD23 | 4                   | 0.43     | 0.08                | 0.42       |
| (1,2100) | 1:25:A:LYS:HG3  | 1:26:A:TYR:HA   | 4                   | 0.28     | 0.12                | 0.28       |
| (1,1565) | 1:22:B:GLU:HB3  | 1:31:B:LYS:HD2  | 4                   | 0.24     | 0.03                | 0.24       |
| (1,2110) | 1:63:B:GLU:HB2  | 1:64:B:ASN:HD21 | 4                   | 0.23     | 0.02                | 0.22       |
| (1,201)  | 1:42:A:SER:H    | 1:1:B:GLY:HA2   | 4                   | 0.21     | 0.05                | 0.18       |
| (1,201)  | 1:42:A:SER:H    | 1:1:B:GLY:HA3   | 4                   | 0.21     | 0.05                | 0.18       |
| (1,2601) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HD3  | 4                   | 0.2      | 0.05                | 0.21       |
| (1,386)  | 1:30:A:LYS:HG3  | 1:65:A:GLY:HA3  | 4                   | 0.2      | 0.05                | 0.2        |
| (1,1623) | 1:30:B:LYS:HE2  | 1:33:B:LEU:HB3  | 4                   | 0.2      | 0.09                | 0.18       |
| (1,479)  | 1:89:A:PHE:HA   | 1:89:A:PHE:HD1  | 4                   | 0.2      | 0.04                | 0.18       |
| (1,454)  | 1:30:A:LYS:HD3  | 1:65:A:GLY:HA2  | 4                   | 0.18     | 0.04                | 0.17       |
| (1,499)  | 1:57:A:VAL:HG21 | 1:81:A:LEU:HG   | 4                   | 0.18     | 0.03                | 0.18       |
| (1,499)  | 1:57:A:VAL:HG22 | 1:81:A:LEU:HG   | 4                   | 0.18     | 0.03                | 0.18       |
| (1,499)  | 1:57:A:VAL:HG23 | 1:81:A:LEU:HG   | 4                   | 0.18     | 0.03                | 0.18       |
| (1,972)  | 1:86:B:ASN:HA   | 1:89:B:PHE:HB2  | 4                   | 0.17     | 0.01                | 0.17       |
| (1,311)  | 1:56:A:LYS:HB2  | 1:56:A:LYS:HD2  | 4                   | 0.16     | 0.03                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1359) | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG3  | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1359) | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG3  | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1359) | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG3  | 4                   | 0.16     | 0.02                | 0.16       |
| (1,144)  | 1:11:A:LEU:HD11 | 1:4:B:LEU:HB2   | 4                   | 0.16     | 0.06                | 0.13       |
| (1,144)  | 1:11:A:LEU:HD12 | 1:4:B:LEU:HB2   | 4                   | 0.16     | 0.06                | 0.13       |
| (1,144)  | 1:11:A:LEU:HD13 | 1:4:B:LEU:HB2   | 4                   | 0.16     | 0.06                | 0.13       |
| (1,3549) | 1:20:B:GLY:HA3  | 1:21:B:LYS:HE2  | 4                   | 0.16     | 0.05                | 0.14       |
| (1,3598) | 1:48:B:GLN:HE22 | 1:49:B:LYS:H    | 4                   | 0.16     | 0.04                | 0.14       |
| (1,832)  | 1:38:A:GLN:HA   | 1:45:A:LEU:HD21 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,832)  | 1:38:A:GLN:HA   | 1:45:A:LEU:HD22 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,832)  | 1:38:A:GLN:HA   | 1:45:A:LEU:HD23 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,3447) | 1:37:A:LEU:HB2  | 1:74:A:TYR:HA   | 4                   | 0.14     | 0.02                | 0.15       |
| (1,1230) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HB2  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG11 | 4                   | 0.13     | 0.02                | 0.14       |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG12 | 4                   | 0.13     | 0.02                | 0.14       |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG13 | 4                   | 0.13     | 0.02                | 0.14       |
| (1,3201) | 1:45:A:LEU:HD11 | 1:46:A:ASP:HB3  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,3201) | 1:45:A:LEU:HD12 | 1:46:A:ASP:HB3  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,3201) | 1:45:A:LEU:HD13 | 1:46:A:ASP:HB3  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,731)  | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,731)  | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,731)  | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1669) | 1:30:A:LYS:HA   | 1:33:A:LEU:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,3617) | 1:63:B:GLU:HA   | 1:66:B:ASP:HB2  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,3415) | 1:16:A:HIS:H    | 1:74:A:TYR:HE2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,241)  | 1:86:A:ASN:HB3  | 1:12:B:ILE:HB   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,298)  | 1:77:B:LEU:HA   | 1:77:B:LEU:HD11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,298)  | 1:77:B:LEU:HA   | 1:77:B:LEU:HD12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,298)  | 1:77:B:LEU:HA   | 1:77:B:LEU:HD13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,253)  | 1:89:A:PHE:HE2  | 1:9:B:GLU:HG2   | 3                   | 1.16     | 0.3                 | 1.2        |
| (1,2319) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HB3  | 3                   | 0.37     | 0.15                | 0.27       |
| (1,1005) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HA   | 3                   | 0.35     | 0.17                | 0.45       |
| (1,856)  | 1:89:B:PHE:HB3  | 1:90:B:TRP:HD1  | 3                   | 0.31     | 0.08                | 0.26       |
| (1,1592) | 1:25:B:LYS:HE3  | 1:26:B:TYR:HE1  | 3                   | 0.3      | 0.19                | 0.18       |
| (1,3231) | 1:75:B:VAL:H    | 1:76:B:VAL:HB   | 3                   | 0.3      | 0.01                | 0.29       |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD21  | 3                   | 0.26     | 0.06                | 0.27       |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD22  | 3                   | 0.26     | 0.06                | 0.27       |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD23  | 3                   | 0.26     | 0.06                | 0.27       |
| (1,2148) | 1:25:B:LYS:HE3  | 1:26:B:TYR:HD1  | 3                   | 0.26     | 0.1                 | 0.3        |
| (1,3422) | 1:22:A:GLU:HB2  | 1:29:A:SER:HA   | 3                   | 0.25     | 0.02                | 0.24       |
| (1,2612) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HD3  | 3                   | 0.24     | 0.06                | 0.26       |
| (1,3382) | 1:37:A:LEU:HA   | 1:40:A:GLU:HG3  | 3                   | 0.22     | 0.12                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2571) | 1:31:B:LYS:HG3  | 1:32:B:GLU:HG3  | 3                   | 0.19     | 0.03                | 0.19       |
| (1,3477) | 1:51:A:VAL:HB   | 1:52:A:ASP:HB3  | 3                   | 0.19     | 0.1                 | 0.13       |
| (1,1278) | 1:89:B:PHE:HB2  | 1:90:B:TRP:HD1  | 3                   | 0.18     | 0.03                | 0.2        |
| (1,3133) | 1:57:A:VAL:H    | 1:58:A:MET:HB3  | 3                   | 0.18     | 0.05                | 0.18       |
| (1,3394) | 1:6:A:THR:HG21  | 1:9:A:GLU:HA    | 3                   | 0.18     | 0.05                | 0.22       |
| (1,3394) | 1:6:A:THR:HG22  | 1:9:A:GLU:HA    | 3                   | 0.18     | 0.05                | 0.22       |
| (1,3394) | 1:6:A:THR:HG23  | 1:9:A:GLU:HA    | 3                   | 0.18     | 0.05                | 0.22       |
| (1,3424) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HE1  | 3                   | 0.18     | 0.07                | 0.14       |
| (1,2401) | 1:1:B:GLY:HA2   | 1:5:B:GLU:HB3   | 3                   | 0.18     | 0.03                | 0.18       |
| (1,3620) | 1:68:B:GLU:HB3  | 1:70:B:ASP:HB3  | 3                   | 0.18     | 0.04                | 0.17       |
| (1,659)  | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG21 | 3                   | 0.18     | 0.08                | 0.15       |
| (1,659)  | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG22 | 3                   | 0.18     | 0.08                | 0.15       |
| (1,659)  | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG23 | 3                   | 0.18     | 0.08                | 0.15       |
| (1,788)  | 1:49:B:LYS:HB3  | 1:49:B:LYS:HE3  | 3                   | 0.17     | 0.02                | 0.16       |
| (1,839)  | 1:38:B:GLN:HA   | 1:45:B:LEU:HD21 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,839)  | 1:38:B:GLN:HA   | 1:45:B:LEU:HD22 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,839)  | 1:38:B:GLN:HA   | 1:45:B:LEU:HD23 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1588) | 1:25:A:LYS:HB2  | 1:25:A:LYS:HE3  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,250)  | 1:86:A:ASN:HD22 | 1:9:B:GLU:HB2   | 3                   | 0.15     | 0.01                | 0.15       |
| (1,1504) | 1:76:B:VAL:HG21 | 1:80:B:ALA:H    | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1504) | 1:76:B:VAL:HG22 | 1:80:B:ALA:H    | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1504) | 1:76:B:VAL:HG23 | 1:80:B:ALA:H    | 3                   | 0.15     | 0.03                | 0.16       |
| (1,391)  | 1:60:B:GLU:HA   | 1:60:B:GLU:HG3  | 3                   | 0.15     | 0.01                | 0.15       |
| (1,3421) | 1:20:A:GLY:HA3  | 1:21:A:LYS:HE2  | 3                   | 0.15     | 0.05                | 0.11       |
| (1,3492) | 1:68:A:GLU:HB3  | 1:70:A:ASP:HB3  | 3                   | 0.14     | 0.04                | 0.13       |
| (1,280)  | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB1  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB2  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB3  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB1  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB2  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB3  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB1  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB2  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB3  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,2917) | 1:19:B:SER:HB2  | 1:28:B:LEU:HB2  | 3                   | 0.14     | 0.03                | 0.12       |
| (1,1221) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HB2  | 3                   | 0.13     | 0.03                | 0.12       |
| (1,435)  | 1:26:B:TYR:HB2  | 1:26:B:TYR:HD2  | 3                   | 0.13     | 0.04                | 0.11       |
| (1,2239) | 1:30:B:LYS:H    | 1:30:B:LYS:HG2  | 3                   | 0.13     | 0.03                | 0.12       |
| (1,3605) | 1:51:B:VAL:HB   | 1:52:B:ASP:HB3  | 3                   | 0.13     | 0.03                | 0.12       |
| (1,3642) | 1:86:B:ASN:HB2  | 1:87:B:ASN:HB2  | 3                   | 0.13     | 0.02                | 0.14       |
| (1,279)  | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB1  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,279)  | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB2  | 3                   | 0.13     | 0.03                | 0.11       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,279)  | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB3  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,279)  | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB1  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,279)  | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB2  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,279)  | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB3  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,279)  | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB1  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,279)  | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB2  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,279)  | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB3  | 3                   | 0.13     | 0.03                | 0.11       |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD21 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD22 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD23 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD21 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD22 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD23 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD21 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD22 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD23 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2082) | 1:25:B:LYS:HG3  | 1:26:B:TYR:H    | 3                   | 0.13     | 0.01                | 0.12       |
| (1,3181) | 1:27:B:LYS:HE3  | 1:71:B:PHE:H    | 3                   | 0.13     | 0.02                | 0.12       |
| (1,621)  | 1:9:A:GLU:HA    | 1:12:A:ILE:HB   | 3                   | 0.12     | 0.01                | 0.13       |
| (1,1606) | 1:83:B:VAL:HG11 | 1:84:B:ALA:H    | 3                   | 0.12     | 0.01                | 0.13       |
| (1,1606) | 1:83:B:VAL:HG12 | 1:84:B:ALA:H    | 3                   | 0.12     | 0.01                | 0.13       |
| (1,1606) | 1:83:B:VAL:HG13 | 1:84:B:ALA:H    | 3                   | 0.12     | 0.01                | 0.13       |
| (1,2234) | 1:30:A:LYS:H    | 1:30:A:LYS:HG2  | 3                   | 0.12     | 0.02                | 0.11       |
| (1,3522) | 1:6:B:THR:HG21  | 1:9:B:GLU:HA    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,3522) | 1:6:B:THR:HG22  | 1:9:B:GLU:HA    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,3522) | 1:6:B:THR:HG23  | 1:9:B:GLU:HA    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,3556) | 1:27:B:LYS:HE3  | 1:69:B:VAL:H    | 3                   | 0.12     | 0.02                | 0.12       |
| (1,129)  | 1:11:A:LEU:HD21 | 1:7:B:ALA:H     | 3                   | 0.12     | 0.01                | 0.12       |
| (1,129)  | 1:11:A:LEU:HD22 | 1:7:B:ALA:H     | 3                   | 0.12     | 0.01                | 0.12       |
| (1,129)  | 1:11:A:LEU:HD23 | 1:7:B:ALA:H     | 3                   | 0.12     | 0.01                | 0.12       |
| (1,951)  | 1:27:A:LYS:HA   | 1:27:A:LYS:HD2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,3552) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HE1  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,299)  | 1:11:A:LEU:HA   | 1:11:A:LEU:HD21 | 3                   | 0.11     | 0.01                | 0.12       |
| (1,299)  | 1:11:A:LEU:HA   | 1:11:A:LEU:HD22 | 3                   | 0.11     | 0.01                | 0.12       |
| (1,299)  | 1:11:A:LEU:HA   | 1:11:A:LEU:HD23 | 3                   | 0.11     | 0.01                | 0.12       |
| (1,209)  | 1:91:A:GLU:HG2  | 1:26:B:TYR:HE1  | 2                   | 0.66     | 0.25                | 0.66       |
| (1,2035) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HB3  | 2                   | 0.58     | 0.16                | 0.58       |
| (1,3539) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB3  | 2                   | 0.34     | 0.08                | 0.34       |
| (1,2517) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG3  | 2                   | 0.32     | 0.14                | 0.32       |
| (1,3177) | 1:27:A:LYS:HE3  | 1:71:A:PHE:H    | 2                   | 0.3      | 0.12                | 0.3        |
| (1,3227) | 1:75:A:VAL:H    | 1:76:A:VAL:HB   | 2                   | 0.29     | 0.02                | 0.29       |
| (1,1833) | 1:25:A:LYS:HB2  | 1:26:A:TYR:HE1  | 2                   | 0.27     | 0.16                | 0.27       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2520) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG3  | 2                   | 0.26     | 0.06                | 0.26       |
| (1,3312) | 1:45:B:LEU:HA   | 1:49:B:LYS:HG2  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,2354) | 1:21:B:LYS:HG3  | 1:32:B:GLU:HB3  | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,3294) | 1:59:A:LYS:H    | 1:61:A:LEU:HD21 | 2                   | 0.24     | 0.06                | 0.24       |
| (1,3294) | 1:59:A:LYS:H    | 1:61:A:LEU:HD22 | 2                   | 0.24     | 0.06                | 0.24       |
| (1,3294) | 1:59:A:LYS:H    | 1:61:A:LEU:HD23 | 2                   | 0.24     | 0.06                | 0.24       |
| (1,348)  | 1:12:B:ILE:HG21 | 1:16:B:HIS:HD2  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,348)  | 1:12:B:ILE:HG22 | 1:16:B:HIS:HD2  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,348)  | 1:12:B:ILE:HG23 | 1:16:B:HIS:HD2  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,1034) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HA   | 2                   | 0.22     | 0.04                | 0.22       |
| (1,277)  | 1:61:A:LEU:HA   | 1:61:A:LEU:HD11 | 2                   | 0.2      | 0.03                | 0.2        |
| (1,277)  | 1:61:A:LEU:HA   | 1:61:A:LEU:HD12 | 2                   | 0.2      | 0.03                | 0.2        |
| (1,277)  | 1:61:A:LEU:HA   | 1:61:A:LEU:HD13 | 2                   | 0.2      | 0.03                | 0.2        |
| (1,3564) | 1:29:B:SER:HA   | 1:31:B:LYS:HE3  | 2                   | 0.2      | 0.08                | 0.2        |
| (1,665)  | 1:39:A:THR:HG21 | 1:40:A:GLU:HG2  | 2                   | 0.2      | 0.09                | 0.2        |
| (1,665)  | 1:39:A:THR:HG22 | 1:40:A:GLU:HG2  | 2                   | 0.2      | 0.09                | 0.2        |
| (1,665)  | 1:39:A:THR:HG23 | 1:40:A:GLU:HG2  | 2                   | 0.2      | 0.09                | 0.2        |
| (1,1530) | 1:24:A:ASP:HB2  | 1:27:A:LYS:HG2  | 2                   | 0.2      | 0.09                | 0.2        |
| (1,3436) | 1:29:A:SER:HA   | 1:31:A:LYS:HE3  | 2                   | 0.19     | 0.08                | 0.19       |
| (1,457)  | 1:30:B:LYS:HD3  | 1:65:B:GLY:HA2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,3367) | 1:13:A:ASN:H    | 1:16:A:HIS:HD2  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,3045) | 1:12:B:ILE:HG21 | 1:16:B:HIS:HE1  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,3045) | 1:12:B:ILE:HG22 | 1:16:B:HIS:HE1  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,3045) | 1:12:B:ILE:HG23 | 1:16:B:HIS:HE1  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,3591) | 1:47:B:ALA:H    | 1:48:B:GLN:HB3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,613)  | 1:25:B:LYS:HG3  | 1:25:B:LYS:HE3  | 2                   | 0.17     | 0.06                | 0.17       |
| (1,389)  | 1:29:B:SER:HB2  | 1:31:B:LYS:HD2  | 2                   | 0.17     | 0.02                | 0.17       |
| (1,688)  | 1:57:B:VAL:HG11 | 1:81:B:LEU:HG   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,688)  | 1:57:B:VAL:HG12 | 1:81:B:LEU:HG   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,688)  | 1:57:B:VAL:HG13 | 1:81:B:LEU:HG   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,853)  | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG2  | 2                   | 0.17     | 0.02                | 0.17       |
| (1,853)  | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG2  | 2                   | 0.17     | 0.02                | 0.17       |
| (1,853)  | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG2  | 2                   | 0.17     | 0.02                | 0.17       |
| (1,2026) | 1:86:B:ASN:HA   | 1:86:B:ASN:HD21 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,3034) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HE1  | 2                   | 0.17     | 0.05                | 0.17       |
| (1,3034) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HE1  | 2                   | 0.17     | 0.05                | 0.17       |
| (1,3034) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HE1  | 2                   | 0.17     | 0.05                | 0.17       |
| (1,385)  | 1:29:A:SER:HB2  | 1:31:A:LYS:HD2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,780)  | 1:49:A:LYS:HB3  | 1:49:A:LYS:HE3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1497) | 1:76:A:VAL:HG21 | 1:80:A:ALA:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1497) | 1:76:A:VAL:HG22 | 1:80:A:ALA:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1497) | 1:76:A:VAL:HG23 | 1:80:A:ALA:H    | 2                   | 0.16     | 0.01                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3553) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HE2  | 2                   | 0.16     | 0.03                | 0.16       |
| (1,3390) | 1:37:B:LEU:HA   | 1:40:B:GLU:HA   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,482)  | 1:89:B:PHE:HA   | 1:89:B:PHE:HD1  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,3648) | 1:92:B:ASN:HB3  | 1:93:B:SER:HB2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,994)  | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG11 | 2                   | 0.15     | 0.01                | 0.15       |
| (1,994)  | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG12 | 2                   | 0.15     | 0.01                | 0.15       |
| (1,994)  | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG13 | 2                   | 0.15     | 0.01                | 0.15       |
| (1,3338) | 1:1:B:GLY:HA3   | 1:5:B:GLU:HB3   | 2                   | 0.15     | 0.01                | 0.15       |
| (1,987)  | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG11 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,987)  | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG12 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,987)  | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG13 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,151)  | 1:80:A:ALA:HA   | 1:72:B:GLN:HA   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,460)  | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,678)  | 1:57:A:VAL:HG11 | 1:81:A:LEU:HG   | 2                   | 0.15     | 0.03                | 0.15       |
| (1,678)  | 1:57:A:VAL:HG12 | 1:81:A:LEU:HG   | 2                   | 0.15     | 0.03                | 0.15       |
| (1,678)  | 1:57:A:VAL:HG13 | 1:81:A:LEU:HG   | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG21 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG22 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG23 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1678) | 1:30:B:LYS:HA   | 1:33:B:LEU:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2881) | 1:46:A:ASP:HB2  | 1:49:A:LYS:HG3  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2304) | 1:29:B:SER:HA   | 1:31:B:LYS:HG2  | 2                   | 0.14     | 0.03                | 0.14       |
| (1,364)  | 1:73:B:GLU:HA   | 1:73:B:GLU:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1275) | 1:21:B:LYS:HB2  | 1:32:B:GLU:HG3  | 2                   | 0.14     | 0.03                | 0.14       |
| (1,2128) | 1:64:B:ASN:HB3  | 1:73:B:GLU:HB2  | 2                   | 0.14     | 0.03                | 0.14       |
| (1,82)   | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB1  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,82)   | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB2  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,82)   | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB3  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,168)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,168)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,168)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,549)  | 1:3:B:GLU:HA    | 1:3:B:GLU:HG2   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1354) | 1:36:A:LEU:HD11 | 1:40:A:GLU:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1354) | 1:36:A:LEU:HD12 | 1:40:A:GLU:HG3  | 2                   | 0.14     | 0.01                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1354) | 1:36:A:LEU:HD13 | 1:40:A:GLU:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,3486) | 1:58:A:MET:HG2  | 1:60:A:GLU:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,7)    | 1:8:A:MET:HE1   | 1:82:B:THR:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (1,7)    | 1:8:A:MET:HE2   | 1:82:B:THR:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (1,7)    | 1:8:A:MET:HE3   | 1:82:B:THR:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (1,242)  | 1:86:A:ASN:HB3  | 1:12:B:ILE:HA   | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,674)  | 1:38:A:GLN:H    | 1:38:A:GLN:HG2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,684)  | 1:38:B:GLN:H    | 1:38:B:GLN:HG2  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,858)  | 1:31:A:LYS:HB3  | 1:31:A:LYS:HE2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,962)  | 1:27:B:LYS:HA   | 1:27:B:LYS:HD2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,3543) | 1:16:B:HIS:H    | 1:74:B:TYR:HE2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,667)  | 1:24:B:ASP:HB3  | 1:27:B:LYS:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1664) | 1:54:B:VAL:HA   | 1:81:B:LEU:HG   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3050) | 1:49:B:LYS:H    | 1:50:B:ASP:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3463) | 1:47:A:ALA:H    | 1:48:A:GLN:HB3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2538) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1234) | 1:91:B:GLU:H    | 1:91:B:GLU:HG2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,600)  | 1:83:B:VAL:H    | 1:83:B:VAL:HG11 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,600)  | 1:83:B:VAL:H    | 1:83:B:VAL:HG12 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,600)  | 1:83:B:VAL:H    | 1:83:B:VAL:HG13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3432) | 1:28:A:LEU:HD21 | 1:35:A:GLU:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3432) | 1:28:A:LEU:HD22 | 1:35:A:GLU:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3432) | 1:28:A:LEU:HD23 | 1:35:A:GLU:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3472) | 1:49:A:LYS:H    | 1:54:A:VAL:HB   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,406)  | 1:72:A:GLN:HA   | 1:75:A:VAL:HG21 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,406)  | 1:72:A:GLN:HA   | 1:75:A:VAL:HG22 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,406)  | 1:72:A:GLN:HA   | 1:75:A:VAL:HG23 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,751)  | 1:51:B:VAL:HG11 | 1:53:B:ALA:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (1,751)  | 1:51:B:VAL:HG12 | 1:53:B:ALA:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (1,751)  | 1:51:B:VAL:HG13 | 1:53:B:ALA:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (1,94)   | 1:75:A:VAL:HG11 | 1:80:B:ALA:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,94)   | 1:75:A:VAL:HG12 | 1:80:B:ALA:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,94)   | 1:75:A:VAL:HG13 | 1:80:B:ALA:HA   | 2                   | 0.11     | 0.0                 | 0.11       |

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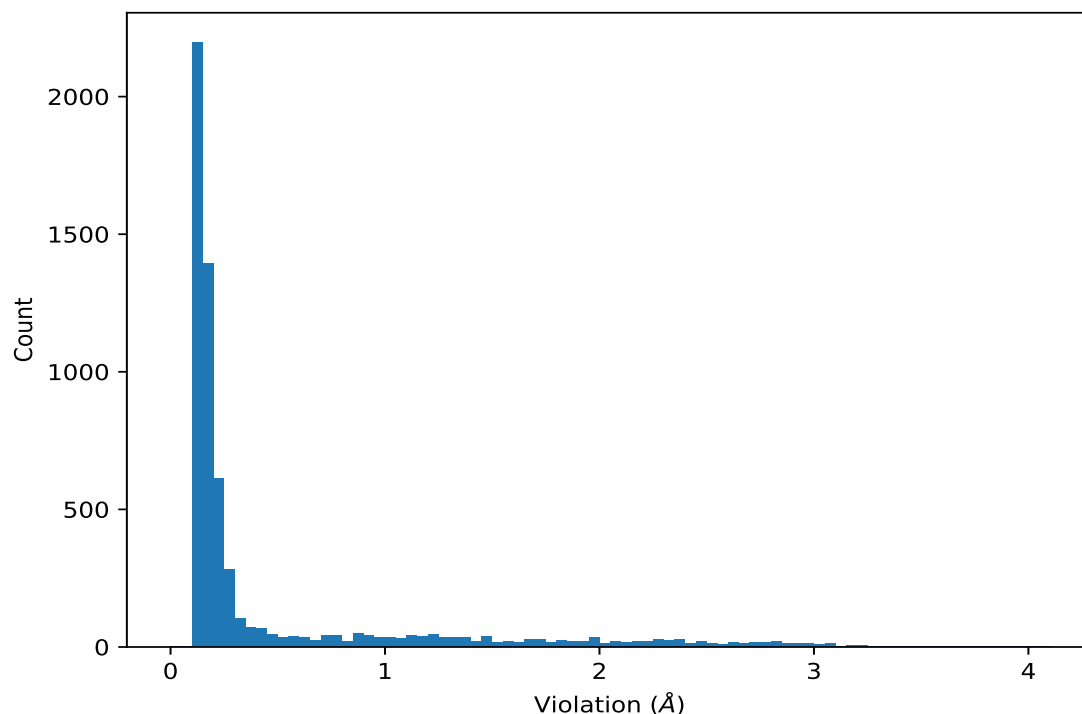
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,859)  | 1:75:A:VAL:H    | 1:75:A:VAL:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,859)  | 1:75:A:VAL:H    | 1:75:A:VAL:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,859)  | 1:75:A:VAL:H    | 1:75:A:VAL:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1269) | 1:41:A:LEU:HD21 | 1:78:A:VAL:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1269) | 1:41:A:LEU:HD22 | 1:78:A:VAL:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1269) | 1:41:A:LEU:HD23 | 1:78:A:VAL:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3405) | 1:14:A:VAL:HA   | 1:74:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1016) | 1:16:B:HIS:HE1 | 1:26:B:TYR:HD1 | 12       | 4.08          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 5        | 4.05          |
| (1,3540) | 1:15:B:PHE:HE2 | 1:26:B:TYR:H   | 20       | 4.02          |
| (1,1010) | 1:16:A:HIS:HE1 | 1:26:A:TYR:HD1 | 17       | 4.02          |
| (1,1010) | 1:16:A:HIS:HE1 | 1:26:A:TYR:HD1 | 19       | 3.73          |
| (1,3412) | 1:15:A:PHE:HE2 | 1:26:A:TYR:H   | 18       | 3.72          |
| (1,1016) | 1:16:B:HIS:HE1 | 1:26:B:TYR:HD1 | 11       | 3.53          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 11       | 3.5           |
| (1,3540) | 1:15:B:PHE:HE2 | 1:26:B:TYR:H   | 11       | 3.48          |
| (1,3540) | 1:15:B:PHE:HE2 | 1:26:B:TYR:H   | 17       | 3.48          |
| (1,3412) | 1:15:A:PHE:HE2 | 1:26:A:TYR:H   | 17       | 3.46          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 8        | 3.38          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE1 | 19       | 3.34          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE2 | 19       | 3.34          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE3 | 19       | 3.34          |
| (1,3540) | 1:15:B:PHE:HE2 | 1:26:B:TYR:H   | 2        | 3.26          |
| (1,3540) | 1:15:B:PHE:HE2 | 1:26:B:TYR:H   | 19       | 3.25          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE1 | 14       | 3.21          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE2 | 14       | 3.21          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE3 | 14       | 3.21          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 1        | 3.2           |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 1        | 3.17          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 1        | 3.17          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 1        | 3.17          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 19       | 3.17          |
| (1,2788) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HA  | 7        | 3.16          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 3        | 3.16          |
| (1,3412) | 1:15:A:PHE:HE2 | 1:26:A:TYR:H   | 12       | 3.15          |
| (1,3540) | 1:15:B:PHE:HE2 | 1:26:B:TYR:H   | 18       | 3.08          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 2        | 3.07          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 2        | 3.07          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 2        | 3.07          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 20       | 3.07          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 20       | 3.07          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 20       | 3.07          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 4        | 3.07          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 7        | 3.07          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 11       | 3.07          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 2        | 3.07          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 12       | 3.06          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE1 | 19       | 3.04          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE2 | 19       | 3.04          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE3 | 19       | 3.04          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 10       | 3.01          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 10       | 3.01          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 17       | 3.01          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 17       | 3.01          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 17       | 3.01          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 16       | 3.01          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 17       | 3.01          |
| (1,2780) | 1:15:A:PHE:HD1 | 1:74:A:TYR:HA  | 17       | 2.99          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1 | 1        | 2.99          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE2 | 1        | 2.99          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE3 | 1        | 2.99          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 15       | 2.99          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 10       | 2.99          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 14       | 2.99          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 3        | 2.98          |
| (1,207)  | 1:91:A:GLU:HB2 | 1:26:B:TYR:HE1 | 8        | 2.98          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1 | 17       | 2.97          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE2 | 17       | 2.97          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE3 | 17       | 2.97          |
| (1,3540) | 1:15:B:PHE:HE2 | 1:26:B:TYR:H   | 7        | 2.96          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 1        | 2.96          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 19       | 2.94          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 19       | 2.94          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 2        | 2.93          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 12       | 2.92          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 12       | 2.92          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 12       | 2.92          |
| (1,2788) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HA  | 18       | 2.91          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE1 | 15       | 2.91          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE2 | 15       | 2.91          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE3 | 15       | 2.91          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 10       | 2.9           |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 18       | 2.89          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 3        | 2.88          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 3        | 2.88          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE1 | 14       | 2.88          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE2 | 14       | 2.88          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE3 | 14       | 2.88          |
| (1,2788) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HA  | 17       | 2.87          |
| (1,2780) | 1:15:A:PHE:HD1 | 1:74:A:TYR:HA  | 18       | 2.87          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 15       | 2.87          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1 | 2        | 2.85          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE2 | 2        | 2.85          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE3 | 2        | 2.85          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1 | 12       | 2.83          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE2 | 12       | 2.83          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE3 | 12       | 2.83          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 4        | 2.82          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 4        | 2.82          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 10       | 2.82          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 10       | 2.82          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 5        | 2.82          |
| (1,2780) | 1:15:A:PHE:HD1 | 1:74:A:TYR:HA  | 7        | 2.81          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 2        | 2.81          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 2        | 2.81          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1 | 20       | 2.81          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE2 | 20       | 2.81          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE3 | 20       | 2.81          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 17       | 2.81          |
| (1,1587) | 1:25:A:LYS:HE3 | 1:26:A:TYR:HE1 | 11       | 2.8           |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE1 | 15       | 2.8           |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE2 | 15       | 2.8           |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE3 | 15       | 2.8           |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 13       | 2.8           |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 5        | 2.79          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 5        | 2.79          |
| (1,204)  | 1:90:A:TRP:HB3 | 1:26:B:TYR:HE1 | 5        | 2.79          |
| (1,3412) | 1:15:A:PHE:HE2 | 1:26:A:TYR:H   | 7        | 2.78          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE1 | 13       | 2.78          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE2 | 13       | 2.78          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE3 | 13       | 2.78          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 13       | 2.78          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 13       | 2.78          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 13       | 2.78          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 4        | 2.78          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 17       | 2.78          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 1        | 2.77          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 1        | 2.77          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2788) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HA  | 2        | 2.76          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 3        | 2.76          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 3        | 2.76          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 9        | 2.74          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 9        | 2.74          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE1 | 9        | 2.74          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE2 | 9        | 2.74          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE3 | 9        | 2.74          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 8        | 2.74          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 10       | 2.74          |
| (1,2788) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HA  | 19       | 2.73          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 10       | 2.73          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 18       | 2.72          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 18       | 2.72          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 2        | 2.72          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 2        | 2.71          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 8        | 2.7           |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 8        | 2.7           |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 8        | 2.7           |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 12       | 2.7           |
| (1,2788) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HA  | 11       | 2.69          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 7        | 2.68          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 7        | 2.68          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 8        | 2.68          |
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 2        | 2.66          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1 | 13       | 2.66          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE2 | 13       | 2.66          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE3 | 13       | 2.66          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 19       | 2.66          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 2        | 2.65          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 13       | 2.65          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 16       | 2.63          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 16       | 2.62          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 16       | 2.62          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 18       | 2.62          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1 | 8        | 2.62          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE2 | 8        | 2.62          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE3 | 8        | 2.62          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 7        | 2.62          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 2        | 2.61          |
| (1,205)  | 1:90:A:TRP:HA  | 1:26:B:TYR:HE1 | 10       | 2.61          |
| (1,204)  | 1:90:A:TRP:HB3 | 1:26:B:TYR:HE1 | 2        | 2.61          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 6        | 2.61          |
| (1,3097) | 1:44:B:PHE:HE2 | 1:85:B:MET:H   | 16       | 2.6           |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 19       | 2.6           |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 16       | 2.6           |
| (1,2780) | 1:15:A:PHE:HD1 | 1:74:A:TYR:HA  | 12       | 2.59          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 18       | 2.59          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 16       | 2.58          |
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 10       | 2.57          |
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 13       | 2.57          |
| (1,2685) | 1:15:B:PHE:HE2 | 1:19:B:SER:HB2 | 20       | 2.56          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 12       | 2.56          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 10       | 2.55          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE1 | 9        | 2.54          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE2 | 9        | 2.54          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE3 | 9        | 2.54          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 6        | 2.54          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 9        | 2.54          |
| (1,2788) | 1:15:B:PHE:HD1 | 1:74:B:TYR:HA  | 20       | 2.52          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 15       | 2.52          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 18       | 2.51          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 7        | 2.5           |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 1        | 2.5           |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 1        | 2.5           |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 11       | 2.49          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 11       | 2.49          |
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 19       | 2.49          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 18       | 2.49          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 17       | 2.48          |
| (1,204)  | 1:90:A:TRP:HB3 | 1:26:B:TYR:HE1 | 11       | 2.48          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 2        | 2.48          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 7        | 2.48          |
| (1,3097) | 1:44:B:PHE:HE2 | 1:85:B:MET:H   | 7        | 2.47          |
| (1,2312) | 1:15:B:PHE:HD2 | 1:26:B:TYR:HA  | 19       | 2.47          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 10       | 2.47          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 19       | 2.47          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 4        | 2.46          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 4        | 2.46          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 3        | 2.46          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 9        | 2.46          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 16       | 2.46          |
| (1,2307) | 1:15:A:PHE:HD2 | 1:26:A:TYR:HA  | 17       | 2.45          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 3        | 2.45          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 17       | 2.44          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 17       | 2.44          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 3        | 2.44          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 15       | 2.43          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 9        | 2.43          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 13       | 2.43          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 5        | 2.42          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 5        | 2.42          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 12       | 2.42          |
| (1,1901) | 1:15:B:PHE:HD2 | 1:19:B:SER:HB2 | 20       | 2.41          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 7        | 2.41          |
| (1,3088) | 1:44:A:PHE:HE2 | 1:85:A:MET:H   | 13       | 2.4           |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 14       | 2.4           |
| (1,3088) | 1:44:A:PHE:HE2 | 1:85:A:MET:H   | 7        | 2.39          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 15       | 2.39          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 15       | 2.39          |
| (1,891)  | 1:44:B:PHE:HE2 | 1:85:B:MET:HB2 | 6        | 2.39          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 13       | 2.39          |
| (1,30)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HE1 | 2        | 2.39          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 18       | 2.38          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 18       | 2.38          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 12       | 2.38          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 20       | 2.38          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 17       | 2.38          |
| (1,30)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HE1 | 10       | 2.38          |
| (1,3128) | 1:86:B:ASN:HB3 | 1:89:B:PHE:HD2 | 5        | 2.37          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 9        | 2.37          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 3        | 2.37          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 1        | 2.37          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 12       | 2.36          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 12       | 2.36          |
| (1,1016) | 1:16:B:HIS:HE1 | 1:26:B:TYR:HD1 | 10       | 2.36          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 17       | 2.36          |
| (1,3088) | 1:44:A:PHE:HE2 | 1:85:A:MET:H   | 11       | 2.35          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1 | 19       | 2.35          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2 | 19       | 2.35          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3 | 19       | 2.35          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 8        | 2.35          |
| (1,30)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HE1 | 19       | 2.35          |
| (1,197)  | 1:44:A:PHE:HD1 | 1:5:B:GLU:HA   | 4        | 2.34          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 18       | 2.34          |
| (1,3088) | 1:44:A:PHE:HE2 | 1:85:A:MET:H   | 4        | 2.33          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 18       | 2.33          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 3        | 2.33          |
| (1,2312) | 1:15:B:PHE:HD2 | 1:26:B:TYR:HA  | 2        | 2.32          |
| (1,2312) | 1:15:B:PHE:HD2 | 1:26:B:TYR:HA  | 20       | 2.32          |
| (1,2136) | 1:25:A:LYS:HE3 | 1:26:A:TYR:HD1 | 11       | 2.32          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 2        | 2.32          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 2        | 2.32          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 8        | 2.32          |
| (1,46)   | 1:8:A:MET:H    | 1:44:B:PHE:HE1 | 16       | 2.32          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 4        | 2.32          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 14       | 2.31          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 14       | 2.31          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 20       | 2.31          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 20       | 2.31          |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 12       | 2.31          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 8        | 2.31          |
| (1,3097) | 1:44:B:PHE:HE2 | 1:85:B:MET:H   | 3        | 2.3           |
| (1,3097) | 1:44:B:PHE:HE2 | 1:85:B:MET:H   | 4        | 2.3           |
| (1,3088) | 1:44:A:PHE:HE2 | 1:85:A:MET:H   | 8        | 2.3           |
| (1,887)  | 1:44:A:PHE:HE2 | 1:85:A:MET:HB2 | 20       | 2.3           |
| (1,3088) | 1:44:A:PHE:HE2 | 1:85:A:MET:H   | 2        | 2.29          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG2 | 8        | 2.29          |
| (1,1513) | 1:44:A:PHE:HE2 | 1:85:A:MET:HG3 | 8        | 2.29          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 4        | 2.29          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 6        | 2.29          |
| (1,198)  | 1:44:A:PHE:HE1 | 1:5:B:GLU:HA   | 2        | 2.29          |
| (1,3097) | 1:44:B:PHE:HE2 | 1:85:B:MET:H   | 2        | 2.28          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 1        | 2.28          |
| (1,1421) | 1:41:A:LEU:HA  | 1:44:A:PHE:HD1 | 11       | 2.28          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE1 | 8        | 2.28          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE2 | 8        | 2.28          |
| (1,1148) | 1:44:B:PHE:HE2 | 1:85:B:MET:HE3 | 8        | 2.28          |
| (1,198)  | 1:44:A:PHE:HE1 | 1:5:B:GLU:HA   | 17       | 2.28          |
| (1,188)  | 1:44:A:PHE:HE1 | 1:8:B:MET:H    | 13       | 2.28          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2 | 16       | 2.27          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3 | 16       | 2.27          |
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 7        | 2.27          |
| (1,2312) | 1:15:B:PHE:HD2 | 1:26:B:TYR:HA  | 17       | 2.26          |
| (1,2307) | 1:15:A:PHE:HD2 | 1:26:A:TYR:HA  | 18       | 2.26          |
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 3        | 2.26          |
| (1,1429) | 1:41:B:LEU:HA  | 1:44:B:PHE:HD1 | 17       | 2.26          |
| (1,29)   | 1:5:A:GLU:HA   | 1:44:B:PHE:HD1 | 6        | 2.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H   | 13       | 2.25          |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1 | 8        | 2.25          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1 | 7        | 2.25          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2 | 7        | 2.25          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3 | 7        | 2.25          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1 | 19       | 2.24          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2 | 19       | 2.24          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3 | 19       | 2.24          |
| (1,197)  | 1:44:A:PHE:HD1  | 1:5:B:GLU:HA   | 20       | 2.24          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H   | 12       | 2.23          |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1 | 12       | 2.23          |
| (1,197)  | 1:44:A:PHE:HD1  | 1:5:B:GLU:HA   | 11       | 2.23          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG2 | 6        | 2.22          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG3 | 6        | 2.22          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG2 | 19       | 2.22          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG3 | 19       | 2.22          |
| (1,46)   | 1:8:A:MET:H     | 1:44:B:PHE:HE1 | 9        | 2.22          |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3 | 20       | 2.21          |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1 | 5        | 2.21          |
| (1,1421) | 1:41:A:LEU:HA   | 1:44:A:PHE:HD1 | 8        | 2.21          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA   | 19       | 2.21          |
| (1,29)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HD1 | 7        | 2.21          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H   | 5        | 2.2           |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1 | 4        | 2.2           |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3 | 11       | 2.19          |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1 | 14       | 2.19          |
| (1,1421) | 1:41:A:LEU:HA   | 1:44:A:PHE:HD1 | 5        | 2.19          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1 | 18       | 2.19          |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA  | 20       | 2.18          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG2 | 19       | 2.18          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG3 | 19       | 2.18          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG2 | 1        | 2.18          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG3 | 1        | 2.18          |
| (1,1421) | 1:41:A:LEU:HA   | 1:44:A:PHE:HD1 | 13       | 2.17          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1 | 19       | 2.16          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1 | 19       | 2.16          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1 | 19       | 2.16          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H   | 3        | 2.16          |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1 | 1        | 2.16          |
| (1,188)  | 1:44:A:PHE:HE1  | 1:8:B:MET:H    | 20       | 2.16          |
| (1,29)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HD1 | 12       | 2.16          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H   | 18       | 2.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1  | 15       | 2.15          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 10       | 2.15          |
| (1,887)  | 1:44:A:PHE:HE2  | 1:85:A:MET:HB2  | 2        | 2.15          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 19       | 2.14          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 19       | 2.14          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 19       | 2.14          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1  | 6        | 2.13          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2  | 6        | 2.13          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3  | 6        | 2.13          |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2  | 19       | 2.13          |
| (1,197)  | 1:44:A:PHE:HD1  | 1:5:B:GLU:HA    | 7        | 2.13          |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 17       | 2.12          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 1        | 2.12          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1  | 13       | 2.12          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2  | 13       | 2.12          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3  | 13       | 2.12          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 16       | 2.12          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 10       | 2.11          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 6        | 2.1           |
| (1,46)   | 1:8:A:MET:H     | 1:44:B:PHE:HE1  | 6        | 2.1           |
| (1,2312) | 1:15:B:PHE:HD2  | 1:26:B:TYR:HA   | 11       | 2.09          |
| (1,2251) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB3  | 17       | 2.09          |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 8        | 2.09          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 8        | 2.09          |
| (1,188)  | 1:44:A:PHE:HE1  | 1:8:B:MET:H     | 1        | 2.09          |
| (1,197)  | 1:44:A:PHE:HD1  | 1:5:B:GLU:HA    | 5        | 2.08          |
| (1,188)  | 1:44:A:PHE:HE1  | 1:8:B:MET:H     | 4        | 2.08          |
| (1,46)   | 1:8:A:MET:H     | 1:44:B:PHE:HE1  | 17       | 2.08          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 5        | 2.07          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 13       | 2.07          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 10       | 2.06          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 17       | 2.06          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 14       | 2.05          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 14       | 2.05          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 14       | 2.05          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 7        | 2.05          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 7        | 2.05          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG13 | 7        | 2.05          |
| (1,46)   | 1:8:A:MET:H     | 1:44:B:PHE:HE1  | 4        | 2.05          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 15       | 2.05          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 19       | 2.04          |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 5        | 2.03          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 6        | 2.03          |
| (1,46)   | 1:8:A:MET:H     | 1:44:B:PHE:HE1  | 12       | 2.03          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 18       | 2.02          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD12 | 18       | 2.02          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD13 | 18       | 2.02          |
| (1,2307) | 1:15:A:PHE:HD2  | 1:26:A:TYR:HA   | 12       | 2.01          |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1  | 16       | 2.01          |
| (1,197)  | 1:44:A:PHE:HD1  | 1:5:B:GLU:HA    | 16       | 2.01          |
| (1,204)  | 1:90:A:TRP:HB3  | 1:26:B:TYR:HE1  | 8        | 2.0           |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 7        | 2.0           |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 12       | 1.99          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 12       | 1.99          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 12       | 1.99          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 17       | 1.99          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD12 | 17       | 1.99          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD13 | 17       | 1.99          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD11 | 17       | 1.99          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD12 | 17       | 1.99          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD13 | 17       | 1.99          |
| (1,2312) | 1:15:B:PHE:HD2  | 1:26:B:TYR:HA   | 18       | 1.99          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG2  | 12       | 1.99          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG3  | 12       | 1.99          |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 12       | 1.99          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 17       | 1.98          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 18       | 1.98          |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1  | 6        | 1.98          |
| (1,197)  | 1:44:A:PHE:HD1  | 1:5:B:GLU:HA    | 1        | 1.98          |
| (1,46)   | 1:8:A:MET:H     | 1:44:B:PHE:HE1  | 5        | 1.98          |
| (1,3125) | 1:86:A:ASN:HB3  | 1:89:A:PHE:HD2  | 19       | 1.97          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD11 | 7        | 1.97          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD12 | 7        | 1.97          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD13 | 7        | 1.97          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 3        | 1.97          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 9        | 1.96          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 9        | 1.96          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 9        | 1.96          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 16       | 1.96          |
| (1,210)  | 1:91:A:GLU:HG3  | 1:26:B:TYR:HE1  | 8        | 1.96          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 13       | 1.96          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG2  | 13       | 1.95          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG3  | 13       | 1.95          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 12       | 1.95          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,29)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HD1  | 5        | 1.95          |
| (1,3125) | 1:86:A:ASN:HB3  | 1:89:A:PHE:HD2  | 15       | 1.94          |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 5        | 1.94          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 2        | 1.93          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD12 | 2        | 1.93          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD13 | 2        | 1.93          |
| (1,2676) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB2  | 18       | 1.93          |
| (1,188)  | 1:44:A:PHE:HE1  | 1:8:B:MET:H     | 5        | 1.93          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 6        | 1.92          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 6        | 1.92          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 6        | 1.92          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 20       | 1.92          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD12 | 20       | 1.92          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD13 | 20       | 1.92          |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3  | 11       | 1.92          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 19       | 1.92          |
| (1,204)  | 1:90:A:TRP:HB3  | 1:26:B:TYR:HE1  | 1        | 1.92          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 7        | 1.92          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 12       | 1.91          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 16       | 1.91          |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2  | 14       | 1.9           |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 11       | 1.9           |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 19       | 1.89          |
| (1,2251) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB3  | 18       | 1.89          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 9        | 1.89          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 18       | 1.89          |
| (1,2685) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB2  | 2        | 1.88          |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 2        | 1.88          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 11       | 1.88          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 14       | 1.88          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 15       | 1.87          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 15       | 1.87          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 15       | 1.87          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 6        | 1.87          |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 1        | 1.87          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 20       | 1.87          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 8        | 1.87          |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3  | 18       | 1.86          |
| (1,204)  | 1:90:A:TRP:HB3  | 1:26:B:TYR:HE1  | 12       | 1.86          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 5        | 1.86          |
| (1,2685) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB2  | 11       | 1.85          |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2  | 13       | 1.85          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,188)  | 1:44:A:PHE:HE1  | 1:8:B:MET:H     | 11       | 1.85          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 1        | 1.84          |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3  | 20       | 1.84          |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2  | 10       | 1.84          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 17       | 1.84          |
| (1,2685) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB2  | 19       | 1.83          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 14       | 1.83          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 14       | 1.82          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 2        | 1.82          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 8        | 1.81          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 3        | 1.81          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 20       | 1.8           |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 11       | 1.8           |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD12 | 11       | 1.8           |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD13 | 11       | 1.8           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG11 | 7        | 1.8           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG12 | 7        | 1.8           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG13 | 7        | 1.8           |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA   | 2        | 1.8           |
| (1,1897) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB2  | 18       | 1.8           |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG2  | 9        | 1.8           |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG3  | 9        | 1.8           |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 15       | 1.8           |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 18       | 1.79          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 18       | 1.79          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG13 | 18       | 1.79          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 17       | 1.78          |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 8        | 1.78          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 4        | 1.78          |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 20       | 1.77          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 13       | 1.77          |
| (1,198)  | 1:44:A:PHE:HE1  | 1:5:B:GLU:HA    | 1        | 1.77          |
| (1,2086) | 1:15:A:PHE:HE2  | 1:26:A:TYR:HA   | 17       | 1.76          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 9        | 1.76          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 1        | 1.76          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 8        | 1.75          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 8        | 1.75          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 8        | 1.75          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 10       | 1.75          |
| (1,2910) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HG2  | 17       | 1.75          |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 11       | 1.74          |
| (1,1901) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB2  | 19       | 1.74          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1 | 9        | 1.74          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1 | 20       | 1.74          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H   | 19       | 1.73          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG2 | 8        | 1.73          |
| (1,1518) | 1:44:B:PHE:HE2  | 1:85:B:MET:HG3 | 8        | 1.73          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1 | 18       | 1.73          |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2 | 5        | 1.73          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1 | 5        | 1.73          |
| (1,2710) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HG  | 7        | 1.72          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1 | 8        | 1.72          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2 | 8        | 1.72          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3 | 8        | 1.72          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1 | 3        | 1.72          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1 | 10       | 1.72          |
| (1,204)  | 1:90:A:TRP:HB3  | 1:26:B:TYR:HE1 | 15       | 1.72          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1 | 20       | 1.71          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1 | 20       | 1.71          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1 | 20       | 1.71          |
| (1,3413) | 1:15:A:PHE:HD2  | 1:19:A:SER:HA  | 17       | 1.71          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H   | 15       | 1.71          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1 | 2        | 1.7           |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1 | 2        | 1.7           |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1 | 2        | 1.7           |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1 | 15       | 1.7           |
| (1,2676) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB2 | 17       | 1.69          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG2 | 6        | 1.69          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG3 | 6        | 1.69          |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3 | 19       | 1.68          |
| (1,887)  | 1:44:A:PHE:HE2  | 1:85:A:MET:HB2 | 18       | 1.68          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1 | 13       | 1.67          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1 | 13       | 1.67          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1 | 13       | 1.67          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H   | 17       | 1.67          |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3 | 7        | 1.67          |
| (1,1901) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB2 | 2        | 1.67          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1 | 12       | 1.67          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1 | 4        | 1.67          |
| (1,3541) | 1:15:B:PHE:HD2  | 1:19:B:SER:HA  | 11       | 1.66          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1 | 9        | 1.66          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1 | 9        | 1.66          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1 | 9        | 1.66          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1 | 17       | 1.66          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 17       | 1.66          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 17       | 1.66          |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD21 | 7        | 1.66          |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD22 | 7        | 1.66          |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD23 | 7        | 1.66          |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA   | 11       | 1.65          |
| (1,2086) | 1:15:A:PHE:HE2  | 1:26:A:TYR:HA   | 18       | 1.65          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 1        | 1.65          |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 12       | 1.65          |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3  | 2        | 1.64          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 19       | 1.63          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 2        | 1.63          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 6        | 1.63          |
| (1,2312) | 1:15:B:PHE:HD2  | 1:26:B:TYR:HA   | 7        | 1.62          |
| (1,2251) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB3  | 12       | 1.62          |
| (1,1992) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB3  | 17       | 1.62          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 16       | 1.61          |
| (1,1897) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB2  | 17       | 1.61          |
| (1,2251) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB3  | 7        | 1.6           |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA   | 19       | 1.6           |
| (1,1429) | 1:41:B:LEU:HA   | 1:44:B:PHE:HD1  | 9        | 1.6           |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD21 | 7        | 1.6           |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD22 | 7        | 1.6           |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD23 | 7        | 1.6           |
| (1,2685) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB2  | 17       | 1.59          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 6        | 1.59          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 6        | 1.59          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 6        | 1.59          |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 2        | 1.59          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 6        | 1.58          |
| (1,1901) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB2  | 11       | 1.58          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 10       | 1.58          |
| (1,2676) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB2  | 12       | 1.57          |
| (1,876)  | 1:15:A:PHE:HD1  | 1:74:A:TYR:HD2  | 17       | 1.57          |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 12       | 1.57          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 16       | 1.56          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 16       | 1.56          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 16       | 1.56          |
| (1,1016) | 1:16:B:HIS:HE1  | 1:26:B:TYR:HD1  | 1        | 1.56          |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 9        | 1.56          |
| (1,29)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HD1  | 9        | 1.56          |
| (1,3541) | 1:15:B:PHE:HD2  | 1:19:B:SER:HA   | 20       | 1.55          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 1        | 1.55          |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 7        | 1.55          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 9        | 1.54          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 12       | 1.54          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 19       | 1.54          |
| (1,3274) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB2  | 11       | 1.53          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 14       | 1.53          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 1        | 1.52          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 1        | 1.52          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 1        | 1.52          |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 17       | 1.52          |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 18       | 1.52          |
| (1,2910) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HG2  | 18       | 1.52          |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 10       | 1.51          |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 15       | 1.51          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1  | 4        | 1.5           |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2  | 4        | 1.5           |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3  | 4        | 1.5           |
| (1,253)  | 1:89:A:PHE:HE2  | 1:9:B:GLU:HG2   | 19       | 1.5           |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD11 | 12       | 1.49          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD12 | 12       | 1.49          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD13 | 12       | 1.49          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG21 | 17       | 1.49          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG22 | 17       | 1.49          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG23 | 17       | 1.49          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 12       | 1.49          |
| (1,1992) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB3  | 18       | 1.48          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD21 | 7        | 1.48          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD22 | 7        | 1.48          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD23 | 7        | 1.48          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG2  | 17       | 1.48          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG3  | 17       | 1.48          |
| (1,3541) | 1:15:B:PHE:HD2  | 1:19:B:SER:HA   | 18       | 1.47          |
| (1,2307) | 1:15:A:PHE:HD2  | 1:26:A:TYR:HA   | 7        | 1.47          |
| (1,1901) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB2  | 17       | 1.47          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 7        | 1.47          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 14       | 1.46          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 7        | 1.46          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD12 | 7        | 1.46          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD13 | 7        | 1.46          |
| (1,2724) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HG   | 7        | 1.46          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 19       | 1.46          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 19       | 1.46          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 19       | 1.46          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG21 | 18       | 1.45          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG22 | 18       | 1.45          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG23 | 18       | 1.45          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG21 | 20       | 1.45          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG22 | 20       | 1.45          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG23 | 20       | 1.45          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1  | 7        | 1.45          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2  | 7        | 1.45          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3  | 7        | 1.45          |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD21 | 7        | 1.45          |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD22 | 7        | 1.45          |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD23 | 7        | 1.45          |
| (1,254)  | 1:89:A:PHE:HD2  | 1:9:B:GLU:HG2   | 19       | 1.45          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 8        | 1.44          |
| (1,1897) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB2  | 12       | 1.44          |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 10       | 1.44          |
| (1,882)  | 1:15:B:PHE:HD1  | 1:74:B:TYR:HD2  | 18       | 1.44          |
| (1,3272) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HB2  | 17       | 1.43          |
| (1,882)  | 1:15:B:PHE:HD1  | 1:74:B:TYR:HD2  | 7        | 1.43          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 17       | 1.42          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 17       | 1.42          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 17       | 1.42          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 1        | 1.42          |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 11       | 1.42          |
| (1,3088) | 1:44:A:PHE:HE2  | 1:85:A:MET:H    | 19       | 1.41          |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA   | 17       | 1.41          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG21 | 11       | 1.41          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG22 | 11       | 1.41          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG23 | 11       | 1.41          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 3        | 1.41          |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD21 | 18       | 1.4           |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD22 | 18       | 1.4           |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD23 | 18       | 1.4           |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 8        | 1.39          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 8        | 1.39          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 8        | 1.39          |
| (1,3413) | 1:15:A:PHE:HD2  | 1:19:A:SER:HA   | 18       | 1.39          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 19       | 1.39          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 19       | 1.39          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 19       | 1.39          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 1        | 1.39          |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 1        | 1.38          |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 11       | 1.38          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 3        | 1.37          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 3        | 1.37          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 3        | 1.37          |
| (1,2724) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HG   | 18       | 1.37          |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3  | 18       | 1.37          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG21 | 12       | 1.37          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG22 | 12       | 1.37          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG23 | 12       | 1.37          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD21 | 18       | 1.37          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD22 | 18       | 1.37          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD23 | 18       | 1.37          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 6        | 1.37          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 4        | 1.37          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 4        | 1.37          |
| (1,882)  | 1:15:B:PHE:HD1  | 1:74:B:TYR:HD2  | 11       | 1.37          |
| (1,2254) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB3  | 17       | 1.36          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 9        | 1.36          |
| (1,3274) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB2  | 20       | 1.35          |
| (1,2685) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB2  | 18       | 1.35          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG21 | 2        | 1.35          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG22 | 2        | 1.35          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG23 | 2        | 1.35          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 13       | 1.35          |
| (1,2086) | 1:15:A:PHE:HE2  | 1:26:A:TYR:HA   | 12       | 1.34          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG21 | 7        | 1.34          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG22 | 7        | 1.34          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG23 | 7        | 1.34          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG21 | 7        | 1.34          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG22 | 7        | 1.34          |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG23 | 7        | 1.34          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1  | 4        | 1.34          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2  | 4        | 1.34          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3  | 4        | 1.34          |
| (1,2710) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HG   | 18       | 1.33          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 6        | 1.33          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 6        | 1.33          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 6        | 1.33          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 10       | 1.33          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 9        | 1.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,946)  | 1:25:B:LYS:HB2  | 1:26:B:TYR:HD1  | 11       | 1.33          |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 5        | 1.32          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1  | 10       | 1.31          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2  | 10       | 1.31          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3  | 10       | 1.31          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD21 | 18       | 1.31          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD22 | 18       | 1.31          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD23 | 18       | 1.31          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 3        | 1.31          |
| (1,882)  | 1:15:B:PHE:HD1  | 1:74:B:TYR:HD2  | 19       | 1.31          |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG11 | 18       | 1.3           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG12 | 18       | 1.3           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG13 | 18       | 1.3           |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 14       | 1.3           |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 14       | 1.3           |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 14       | 1.3           |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 8        | 1.3           |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 17       | 1.3           |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3  | 2        | 1.29          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 20       | 1.29          |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 8        | 1.29          |
| (1,882)  | 1:15:B:PHE:HD1  | 1:74:B:TYR:HD2  | 17       | 1.29          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 4        | 1.28          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 4        | 1.28          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 4        | 1.28          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 10       | 1.28          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 10       | 1.28          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 10       | 1.28          |
| (1,2949) | 1:15:B:PHE:HE2  | 1:19:B:SER:HA   | 11       | 1.28          |
| (1,882)  | 1:15:B:PHE:HD1  | 1:74:B:TYR:HD2  | 2        | 1.28          |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 5        | 1.28          |
| (1,1901) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB2  | 18       | 1.27          |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD21 | 12       | 1.27          |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD22 | 12       | 1.27          |
| (1,1667) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HD23 | 12       | 1.27          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 15       | 1.27          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 2        | 1.27          |
| (1,3413) | 1:15:A:PHE:HD2  | 1:19:A:SER:HA   | 12       | 1.26          |
| (1,2910) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HG2  | 12       | 1.26          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 11       | 1.26          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 11       | 1.26          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG13 | 11       | 1.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD11 | 18       | 1.25          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD12 | 18       | 1.25          |
| (1,3065) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD13 | 18       | 1.25          |
| (1,2938) | 1:15:A:PHE:HE2  | 1:19:A:SER:HA   | 17       | 1.25          |
| (1,2676) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB2  | 7        | 1.25          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 13       | 1.25          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 13       | 1.25          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 13       | 1.25          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 9        | 1.25          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 10       | 1.25          |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 14       | 1.25          |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 20       | 1.25          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 8        | 1.24          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 8        | 1.24          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 8        | 1.24          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 16       | 1.24          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 16       | 1.24          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 16       | 1.24          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 18       | 1.24          |
| (1,887)  | 1:44:A:PHE:HE2  | 1:85:A:MET:HB2  | 6        | 1.24          |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1  | 9        | 1.23          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 2        | 1.23          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 2        | 1.23          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 2        | 1.23          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 9        | 1.23          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 9        | 1.23          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 9        | 1.23          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 20       | 1.23          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 20       | 1.23          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 20       | 1.23          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG2  | 13       | 1.23          |
| (1,1513) | 1:44:A:PHE:HE2  | 1:85:A:MET:HG3  | 13       | 1.23          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 1        | 1.23          |
| (1,876)  | 1:15:A:PHE:HD1  | 1:74:A:TYR:HD2  | 7        | 1.23          |
| (1,254)  | 1:89:A:PHE:HD2  | 1:9:B:GLU:HG2   | 15       | 1.23          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 1        | 1.22          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 1        | 1.22          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 1        | 1.22          |
| (1,2949) | 1:15:B:PHE:HE2  | 1:19:B:SER:HA   | 20       | 1.22          |
| (1,2685) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB2  | 7        | 1.22          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD21 | 2        | 1.22          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD22 | 2        | 1.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD23 | 2        | 1.22          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 16       | 1.22          |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3  | 19       | 1.21          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 4        | 1.21          |
| (1,2724) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HG   | 17       | 1.2           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG11 | 17       | 1.2           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG12 | 17       | 1.2           |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG13 | 17       | 1.2           |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 12       | 1.2           |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 12       | 1.2           |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 12       | 1.2           |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD21 | 12       | 1.2           |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD22 | 12       | 1.2           |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD23 | 12       | 1.2           |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 11       | 1.2           |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 1        | 1.2           |
| (1,253)  | 1:89:A:PHE:HE2  | 1:9:B:GLU:HG2   | 15       | 1.2           |
| (1,2910) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HG2  | 7        | 1.19          |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG11 | 12       | 1.19          |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG12 | 12       | 1.19          |
| (1,2580) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG13 | 12       | 1.19          |
| (1,882)  | 1:15:B:PHE:HD1  | 1:74:B:TYR:HD2  | 20       | 1.19          |
| (1,204)  | 1:90:A:TRP:HB3  | 1:26:B:TYR:HE1  | 10       | 1.19          |
| (1,203)  | 1:90:A:TRP:HB2  | 1:26:B:TYR:HE1  | 5        | 1.19          |
| (1,2724) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HG   | 2        | 1.18          |
| (1,1901) | 1:15:B:PHE:HD2  | 1:19:B:SER:HB2  | 7        | 1.18          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 3        | 1.18          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 3        | 1.18          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 3        | 1.18          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 3        | 1.18          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 8        | 1.18          |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 10       | 1.18          |
| (1,1992) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB3  | 12       | 1.17          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD21 | 17       | 1.17          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD22 | 17       | 1.17          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD23 | 17       | 1.17          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 4        | 1.17          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 8        | 1.17          |
| (1,1992) | 1:15:A:PHE:HE2  | 1:19:A:SER:HB3  | 7        | 1.16          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 10       | 1.16          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 10       | 1.16          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 10       | 1.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,876)  | 1:15:A:PHE:HD1  | 1:74:A:TYR:HD2  | 12       | 1.16          |
| (1,876)  | 1:15:A:PHE:HD1  | 1:74:A:TYR:HD2  | 18       | 1.16          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 10       | 1.15          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 10       | 1.15          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 10       | 1.15          |
| (1,2287) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HD2  | 17       | 1.15          |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA   | 18       | 1.15          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 15       | 1.15          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 15       | 1.15          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 15       | 1.15          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 2        | 1.15          |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2  | 8        | 1.15          |
| (1,254)  | 1:89:A:PHE:HD2  | 1:9:B:GLU:HG2   | 11       | 1.15          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG21 | 17       | 1.14          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG22 | 17       | 1.14          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG23 | 17       | 1.14          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 12       | 1.14          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 9        | 1.14          |
| (1,3274) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB2  | 17       | 1.13          |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 2        | 1.13          |
| (1,2091) | 1:15:B:PHE:HE2  | 1:26:B:TYR:HA   | 7        | 1.13          |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3  | 7        | 1.13          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 20       | 1.13          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 12       | 1.12          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 12       | 1.12          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 12       | 1.12          |
| (1,2710) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HG   | 12       | 1.12          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 2        | 1.12          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 2        | 1.12          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG13 | 2        | 1.12          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 19       | 1.12          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 19       | 1.12          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG13 | 19       | 1.12          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 1        | 1.12          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 1        | 1.12          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 1        | 1.12          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 17       | 1.12          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD21 | 2        | 1.12          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD22 | 2        | 1.12          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD23 | 2        | 1.12          |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD21 | 18       | 1.12          |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD22 | 18       | 1.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD23 | 18       | 1.12          |
| (1,206)  | 1:91:A:GLU:H    | 1:26:B:TYR:HD1  | 2        | 1.12          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 3        | 1.11          |
| (1,946)  | 1:25:B:LYS:HB2  | 1:26:B:TYR:HD1  | 1        | 1.11          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 20       | 1.1           |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 20       | 1.1           |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG13 | 20       | 1.1           |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG21 | 18       | 1.1           |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG22 | 18       | 1.1           |
| (1,1961) | 1:15:A:PHE:HD1  | 1:69:A:VAL:HG23 | 18       | 1.1           |
| (1,1897) | 1:15:A:PHE:HD2  | 1:19:A:SER:HB2  | 7        | 1.1           |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 6        | 1.09          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 6        | 1.09          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 6        | 1.09          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 11       | 1.09          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 11       | 1.09          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 11       | 1.09          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD21 | 19       | 1.09          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD22 | 19       | 1.09          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD23 | 19       | 1.09          |
| (1,891)  | 1:44:B:PHE:HE2  | 1:85:B:MET:HB2  | 9        | 1.09          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 16       | 1.08          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 16       | 1.08          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 5        | 1.08          |
| (1,946)  | 1:25:B:LYS:HB2  | 1:26:B:TYR:HD1  | 10       | 1.08          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 7        | 1.07          |
| (1,3413) | 1:15:A:PHE:HD2  | 1:19:A:SER:HA   | 7        | 1.06          |
| (1,2938) | 1:15:A:PHE:HE2  | 1:19:A:SER:HA   | 18       | 1.06          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 3        | 1.06          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 3        | 1.06          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 11       | 1.06          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 1        | 1.06          |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 10       | 1.06          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 2        | 1.05          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 2        | 1.05          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 2        | 1.05          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG11 | 7        | 1.05          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG12 | 7        | 1.05          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG13 | 7        | 1.05          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 1        | 1.05          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 12       | 1.05          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 18       | 1.04          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3274) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB2  | 18       | 1.03          |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1  | 10       | 1.03          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG21 | 19       | 1.03          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG22 | 19       | 1.03          |
| (1,1966) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG23 | 19       | 1.03          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 10       | 1.03          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 10       | 1.03          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 10       | 1.03          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 5        | 1.02          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 5        | 1.02          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 5        | 1.02          |
| (1,2724) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HG   | 19       | 1.02          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 18       | 1.02          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 18       | 1.02          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 18       | 1.02          |
| (1,30)   | 1:5:A:GLU:HA    | 1:44:B:PHE:HE1  | 9        | 1.02          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 7        | 1.01          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 7        | 1.01          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 7        | 1.01          |
| (1,2294) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HD2  | 19       | 1.01          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 2        | 1.01          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 2        | 1.01          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 2        | 1.01          |
| (1,1401) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HD1  | 5        | 1.01          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 5        | 1.01          |
| (1,976)  | 1:41:A:LEU:HG   | 1:44:A:PHE:HD1  | 13       | 1.01          |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG11 | 17       | 1.0           |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG12 | 17       | 1.0           |
| (1,2589) | 1:15:B:PHE:HD1  | 1:69:B:VAL:HG13 | 17       | 1.0           |
| (1,2294) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HD2  | 11       | 1.0           |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1  | 16       | 1.0           |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2  | 16       | 1.0           |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3  | 16       | 1.0           |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 7        | 1.0           |
| (1,3541) | 1:15:B:PHE:HD2  | 1:19:B:SER:HA   | 7        | 0.99          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG11 | 7        | 0.99          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG12 | 7        | 0.99          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG13 | 7        | 0.99          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD21 | 20       | 0.99          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD22 | 20       | 0.99          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD23 | 20       | 0.99          |
| (1,3067) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD11 | 19       | 0.98          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3067) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD12 | 19       | 0.98          |
| (1,3067) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD13 | 19       | 0.98          |
| (1,2949) | 1:15:B:PHE:HE2 | 1:19:B:SER:HA   | 18       | 0.98          |
| (1,2294) | 1:15:B:PHE:HE1 | 1:74:B:TYR:HD2  | 7        | 0.98          |
| (1,1944) | 1:44:A:PHE:HD2 | 1:85:A:MET:HG2  | 10       | 0.98          |
| (1,1944) | 1:44:A:PHE:HD2 | 1:85:A:MET:HG3  | 10       | 0.98          |
| (1,1401) | 1:41:A:LEU:HB3 | 1:44:A:PHE:HD1  | 13       | 0.98          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE1  | 10       | 0.98          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE2  | 10       | 0.98          |
| (1,1106) | 1:44:B:PHE:HD2 | 1:85:B:MET:HE3  | 10       | 0.98          |
| (1,3274) | 1:15:B:PHE:HE2 | 1:27:B:LYS:HB2  | 2        | 0.97          |
| (1,3274) | 1:15:B:PHE:HE2 | 1:27:B:LYS:HB2  | 19       | 0.97          |
| (1,3272) | 1:15:A:PHE:HE2 | 1:27:A:LYS:HB2  | 12       | 0.97          |
| (1,2321) | 1:25:A:LYS:HA  | 1:26:A:TYR:HD1  | 20       | 0.97          |
| (1,976)  | 1:41:A:LEU:HG  | 1:44:A:PHE:HD1  | 5        | 0.97          |
| (1,892)  | 1:44:B:PHE:HE2 | 1:82:B:THR:HA   | 7        | 0.97          |
| (1,892)  | 1:44:B:PHE:HE2 | 1:82:B:THR:HA   | 16       | 0.97          |
| (1,515)  | 1:44:B:PHE:HA  | 1:44:B:PHE:HD2  | 14       | 0.97          |
| (1,1944) | 1:44:A:PHE:HD2 | 1:85:A:MET:HG2  | 7        | 0.96          |
| (1,1944) | 1:44:A:PHE:HD2 | 1:85:A:MET:HG3  | 7        | 0.96          |
| (1,3541) | 1:15:B:PHE:HD2 | 1:19:B:SER:HA   | 2        | 0.95          |
| (1,3105) | 1:15:B:PHE:HE1 | 1:70:B:ASP:HB3  | 18       | 0.95          |
| (1,1944) | 1:44:A:PHE:HD2 | 1:85:A:MET:HG2  | 4        | 0.95          |
| (1,1944) | 1:44:A:PHE:HD2 | 1:85:A:MET:HG3  | 4        | 0.95          |
| (1,1406) | 1:41:B:LEU:HB3 | 1:44:B:PHE:HD1  | 6        | 0.95          |
| (1,3541) | 1:15:B:PHE:HD2 | 1:19:B:SER:HA   | 19       | 0.94          |
| (1,2331) | 1:25:B:LYS:HA  | 1:26:B:TYR:HD1  | 10       | 0.94          |
| (1,2331) | 1:25:B:LYS:HA  | 1:26:B:TYR:HD1  | 11       | 0.94          |
| (1,2294) | 1:15:B:PHE:HE1 | 1:74:B:TYR:HD2  | 17       | 0.94          |
| (1,2294) | 1:15:B:PHE:HE1 | 1:74:B:TYR:HD2  | 18       | 0.94          |
| (1,1667) | 1:15:A:PHE:HE1 | 1:28:A:LEU:HD21 | 17       | 0.94          |
| (1,1667) | 1:15:A:PHE:HE1 | 1:28:A:LEU:HD22 | 17       | 0.94          |
| (1,1667) | 1:15:A:PHE:HE1 | 1:28:A:LEU:HD23 | 17       | 0.94          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG2  | 7        | 0.94          |
| (1,1518) | 1:44:B:PHE:HE2 | 1:85:B:MET:HG3  | 7        | 0.94          |
| (1,515)  | 1:44:B:PHE:HA  | 1:44:B:PHE:HD2  | 19       | 0.94          |
| (1,511)  | 1:44:A:PHE:HA  | 1:44:A:PHE:HD2  | 6        | 0.94          |
| (1,2321) | 1:25:A:LYS:HA  | 1:26:A:TYR:HD1  | 14       | 0.93          |
| (1,1058) | 1:15:B:PHE:HD1 | 1:28:B:LEU:HD21 | 17       | 0.93          |
| (1,1058) | 1:15:B:PHE:HD1 | 1:28:B:LEU:HD22 | 17       | 0.93          |
| (1,1058) | 1:15:B:PHE:HD1 | 1:28:B:LEU:HD23 | 17       | 0.93          |
| (1,2294) | 1:15:B:PHE:HE1 | 1:74:B:TYR:HD2  | 2        | 0.92          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2287) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HD2 | 7        | 0.92          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2 | 9        | 0.92          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3 | 9        | 0.92          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1 | 18       | 0.92          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2 | 18       | 0.92          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3 | 18       | 0.92          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2 | 8        | 0.92          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2 | 12       | 0.92          |
| (1,2000) | 1:15:B:PHE:HE2  | 1:19:B:SER:HB3 | 17       | 0.91          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1 | 7        | 0.91          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1 | 7        | 0.91          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1 | 7        | 0.91          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1 | 12       | 0.91          |
| (1,209)  | 1:91:A:GLU:HG2  | 1:26:B:TYR:HE1 | 2        | 0.91          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1 | 18       | 0.9           |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1 | 18       | 0.9           |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1 | 18       | 0.9           |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1 | 3        | 0.9           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2 | 1        | 0.9           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3 | 1        | 0.9           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2 | 3        | 0.9           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3 | 3        | 0.9           |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1 | 17       | 0.9           |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1 | 17       | 0.9           |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1 | 17       | 0.9           |
| (1,1810) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HE2 | 19       | 0.9           |
| (1,2287) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HD2 | 18       | 0.89          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1 | 9        | 0.89          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1 | 9        | 0.89          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1 | 9        | 0.89          |
| (1,946)  | 1:25:B:LYS:HB2  | 1:26:B:TYR:HD1 | 2        | 0.89          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1 | 1        | 0.89          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1 | 17       | 0.88          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1 | 17       | 0.88          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1 | 17       | 0.88          |
| (1,2710) | 1:15:A:PHE:HE1  | 1:28:A:LEU:HG  | 17       | 0.88          |
| (1,2331) | 1:25:B:LYS:HA   | 1:26:B:TYR:HD1 | 1        | 0.88          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1 | 12       | 0.88          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2 | 12       | 0.88          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3 | 12       | 0.88          |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1 | 11       | 0.88          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1 | 16       | 0.88          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 11       | 0.88          |
| (1,3272) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HB2  | 18       | 0.87          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 16       | 0.87          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 18       | 0.87          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD21 | 20       | 0.87          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD22 | 20       | 0.87          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD23 | 20       | 0.87          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 13       | 0.87          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 19       | 0.87          |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 12       | 0.86          |
| (1,2086) | 1:15:A:PHE:HE2  | 1:26:A:TYR:HA   | 7        | 0.86          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 17       | 0.86          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 17       | 0.86          |
| (1,1810) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HE2  | 7        | 0.86          |
| (1,1810) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HE2  | 11       | 0.86          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD21 | 11       | 0.86          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD22 | 11       | 0.86          |
| (1,1676) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HD23 | 11       | 0.86          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD21 | 11       | 0.86          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD22 | 11       | 0.86          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD23 | 11       | 0.86          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 15       | 0.86          |
| (1,203)  | 1:90:A:TRP:HB2  | 1:26:B:TYR:HE1  | 8        | 0.86          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 16       | 0.85          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 16       | 0.85          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 16       | 0.85          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 4        | 0.85          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 4        | 0.85          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 4        | 0.85          |
| (1,982)  | 1:41:B:LEU:HG   | 1:44:B:PHE:HD1  | 6        | 0.85          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 1        | 0.85          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 20       | 0.85          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 2        | 0.85          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 10       | 0.85          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG11 | 18       | 0.84          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG12 | 18       | 0.84          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG13 | 18       | 0.84          |
| (1,1810) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HE2  | 2        | 0.84          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 11       | 0.82          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 11       | 0.82          |
| (1,1800) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HE2  | 17       | 0.82          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 17       | 0.82          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2528) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB3  | 7        | 0.81          |
| (1,2522) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB3  | 17       | 0.81          |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1  | 8        | 0.81          |
| (1,3274) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB2  | 7        | 0.8           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 10       | 0.8           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 10       | 0.8           |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 5        | 0.8           |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 5        | 0.8           |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD21 | 17       | 0.8           |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD22 | 17       | 0.8           |
| (1,1051) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HD23 | 17       | 0.8           |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 3        | 0.79          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 3        | 0.79          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 3        | 0.79          |
| (1,2938) | 1:15:A:PHE:HE2  | 1:19:A:SER:HA   | 12       | 0.79          |
| (1,2294) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HD2  | 20       | 0.79          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 5        | 0.79          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 5        | 0.79          |
| (1,1800) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HE2  | 12       | 0.79          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 8        | 0.79          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 5        | 0.79          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 15       | 0.79          |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1  | 1        | 0.78          |
| (1,2287) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HD2  | 12       | 0.78          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 4        | 0.78          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 4        | 0.78          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 4        | 0.78          |
| (1,1810) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HE2  | 18       | 0.78          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 5        | 0.77          |
| (1,2724) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HG   | 11       | 0.77          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD21 | 19       | 0.77          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD22 | 19       | 0.77          |
| (1,1058) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HD23 | 19       | 0.77          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 7        | 0.77          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 13       | 0.77          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 10       | 0.77          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 16       | 0.77          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 8        | 0.77          |
| (1,253)  | 1:89:A:PHE:HE2  | 1:9:B:GLU:HG2   | 11       | 0.77          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 18       | 0.76          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 18       | 0.76          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 18       | 0.76          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3272) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HB2  | 7        | 0.76          |
| (1,2205) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB2  | 7        | 0.76          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 18       | 0.76          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 18       | 0.76          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 18       | 0.76          |
| (1,2035) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HB3  | 7        | 0.75          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1  | 16       | 0.75          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2  | 16       | 0.75          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3  | 16       | 0.75          |
| (1,3125) | 1:86:A:ASN:HB3  | 1:89:A:PHE:HD2  | 11       | 0.74          |
| (1,2938) | 1:15:A:PHE:HE2  | 1:19:A:SER:HA   | 7        | 0.74          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG21 | 7        | 0.74          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG22 | 7        | 0.74          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG23 | 7        | 0.74          |
| (1,208)  | 1:91:A:GLU:HB3  | 1:26:B:TYR:HE1  | 15       | 0.74          |
| (1,2724) | 1:15:B:PHE:HE1  | 1:28:B:LEU:HG   | 20       | 0.73          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 3        | 0.73          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 3        | 0.73          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 3        | 0.73          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 8        | 0.73          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 8        | 0.73          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 8        | 0.73          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 13       | 0.72          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 13       | 0.72          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 13       | 0.72          |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 3        | 0.72          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 9        | 0.72          |
| (1,2198) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB2  | 18       | 0.71          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD21 | 19       | 0.71          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD22 | 19       | 0.71          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD23 | 19       | 0.71          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 18       | 0.71          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 18       | 0.71          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 18       | 0.71          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 18       | 0.71          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 18       | 0.71          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 11       | 0.71          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 11       | 0.71          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 11       | 0.71          |
| (1,1800) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HE2  | 18       | 0.71          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG21 | 17       | 0.71          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG22 | 17       | 0.71          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG23 | 17       | 0.71          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 5        | 0.71          |
| (1,1406) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HD1  | 7        | 0.71          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 5        | 0.71          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 12       | 0.71          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 4        | 0.7           |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 4        | 0.7           |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 4        | 0.7           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 4        | 0.7           |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 4        | 0.7           |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 16       | 0.69          |
| (1,2916) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HG2  | 19       | 0.69          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 11       | 0.69          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 11       | 0.69          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 11       | 0.69          |
| (1,1016) | 1:16:B:HIS:HE1  | 1:26:B:TYR:HD1  | 5        | 0.69          |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1  | 11       | 0.68          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 18       | 0.68          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 18       | 0.68          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 19       | 0.68          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 19       | 0.68          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1  | 12       | 0.68          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2  | 12       | 0.68          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3  | 12       | 0.68          |
| (1,1810) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HE2  | 20       | 0.67          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1  | 11       | 0.67          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2  | 11       | 0.67          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3  | 11       | 0.67          |
| (1,3105) | 1:15:B:PHE:HE1  | 1:70:B:ASP:HB3  | 2        | 0.66          |
| (1,2522) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB3  | 18       | 0.66          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 16       | 0.66          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 16       | 0.66          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 16       | 0.66          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 4        | 0.65          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 1        | 0.64          |
| (1,3516) | 1:89:A:PHE:H    | 1:89:A:PHE:HE2  | 1        | 0.64          |
| (1,2331) | 1:25:B:LYS:HA   | 1:26:B:TYR:HD1  | 2        | 0.64          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD21 | 18       | 0.64          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD22 | 18       | 0.64          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD23 | 18       | 0.64          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 12       | 0.64          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 12       | 0.64          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 12       | 0.64          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG21 | 18       | 0.64          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG22 | 18       | 0.64          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG23 | 18       | 0.64          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 4        | 0.64          |
| (1,3105) | 1:15:B:PHE:HE1  | 1:70:B:ASP:HB3  | 17       | 0.63          |
| (1,2949) | 1:15:B:PHE:HE2  | 1:19:B:SER:HA   | 2        | 0.63          |
| (1,2205) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB2  | 17       | 0.63          |
| (1,2198) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB2  | 7        | 0.63          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG11 | 18       | 0.63          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG12 | 18       | 0.63          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG13 | 18       | 0.63          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 10       | 0.63          |
| (1,2522) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB3  | 7        | 0.62          |
| (1,1810) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HE2  | 17       | 0.62          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 11       | 0.62          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 17       | 0.62          |
| (1,3101) | 1:15:A:PHE:HE1  | 1:70:A:ASP:HB3  | 18       | 0.61          |
| (1,3516) | 1:89:A:PHE:H    | 1:89:A:PHE:HE2  | 20       | 0.6           |
| (1,2528) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB3  | 17       | 0.6           |
| (1,2528) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB3  | 18       | 0.6           |
| (1,2329) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HB3  | 7        | 0.6           |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 9        | 0.6           |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 9        | 0.6           |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 9        | 0.6           |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 11       | 0.6           |
| (1,210)  | 1:91:A:GLU:HG3  | 1:26:B:TYR:HE1  | 5        | 0.6           |
| (1,3101) | 1:15:A:PHE:HE1  | 1:70:A:ASP:HB3  | 12       | 0.59          |
| (1,2198) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB2  | 17       | 0.59          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG2  | 2        | 0.59          |
| (1,1944) | 1:44:A:PHE:HD2  | 1:85:A:MET:HG3  | 2        | 0.59          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG21 | 20       | 0.59          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG22 | 20       | 0.59          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG23 | 20       | 0.59          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG21 | 18       | 0.59          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG22 | 18       | 0.59          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG23 | 18       | 0.59          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 5        | 0.59          |
| (1,2319) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HB3  | 17       | 0.58          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 6        | 0.58          |
| (1,3101) | 1:15:A:PHE:HE1  | 1:70:A:ASP:HB3  | 17       | 0.57          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 1        | 0.57          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 1        | 0.57          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 1        | 0.57          |
| (1,203)  | 1:90:A:TRP:HB2  | 1:26:B:TYR:HE1  | 11       | 0.57          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 5        | 0.56          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 5        | 0.56          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 5        | 0.56          |
| (1,2528) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB3  | 19       | 0.56          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 13       | 0.56          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 13       | 0.56          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 13       | 0.56          |
| (1,1800) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HE2  | 7        | 0.56          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG21 | 7        | 0.56          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG22 | 7        | 0.56          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG23 | 7        | 0.56          |
| (1,1592) | 1:25:B:LYS:HE3  | 1:26:B:TYR:HE1  | 15       | 0.56          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD21 | 7        | 0.55          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD22 | 7        | 0.55          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD23 | 7        | 0.55          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 16       | 0.55          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 16       | 0.55          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG21 | 17       | 0.55          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG22 | 17       | 0.55          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG23 | 17       | 0.55          |
| (1,2949) | 1:15:B:PHE:HE2  | 1:19:B:SER:HA   | 19       | 0.54          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG21 | 2        | 0.54          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG22 | 2        | 0.54          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG23 | 2        | 0.54          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 3        | 0.54          |
| (1,3541) | 1:15:B:PHE:HD2  | 1:19:B:SER:HA   | 17       | 0.53          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1  | 5        | 0.53          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1  | 5        | 0.53          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1  | 5        | 0.53          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1  | 5        | 0.53          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2  | 5        | 0.53          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3  | 5        | 0.53          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 1        | 0.53          |
| (1,2528) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB3  | 11       | 0.52          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD21 | 2        | 0.52          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD22 | 2        | 0.52          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD23 | 2        | 0.52          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD21 | 20       | 0.52          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD22 | 20       | 0.52          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD23 | 20       | 0.52          |
| (1,1824) | 1:41:A:LEU:HD11 | 1:44:A:PHE:HD1  | 5        | 0.52          |
| (1,1824) | 1:41:A:LEU:HD12 | 1:44:A:PHE:HD1  | 5        | 0.52          |
| (1,1824) | 1:41:A:LEU:HD13 | 1:44:A:PHE:HD1  | 5        | 0.52          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG21 | 11       | 0.52          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG22 | 11       | 0.52          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG23 | 11       | 0.52          |
| (1,2028) | 1:15:A:PHE:HD1  | 1:28:A:LEU:HB3  | 7        | 0.51          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 4        | 0.51          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 8        | 0.51          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 9        | 0.5           |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1  | 10       | 0.5           |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2  | 10       | 0.5           |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3  | 10       | 0.5           |
| (1,210)  | 1:91:A:GLU:HG3  | 1:26:B:TYR:HE1  | 12       | 0.5           |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2  | 6        | 0.49          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG21 | 12       | 0.49          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG22 | 12       | 0.49          |
| (1,1687) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG23 | 12       | 0.49          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE2  | 9        | 0.49          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE3  | 9        | 0.49          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 15       | 0.48          |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2  | 15       | 0.48          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 2        | 0.48          |
| (1,3484) | 1:57:A:VAL:H    | 1:58:A:MET:HG2  | 1        | 0.48          |
| (1,3484) | 1:57:A:VAL:H    | 1:58:A:MET:HG2  | 7        | 0.48          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 13       | 0.48          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 8        | 0.48          |
| (1,2528) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB3  | 2        | 0.48          |
| (1,1352) | 1:39:B:THR:HG21 | 1:40:B:GLU:HA   | 15       | 0.48          |
| (1,1352) | 1:39:B:THR:HG22 | 1:40:B:GLU:HA   | 15       | 0.48          |
| (1,1352) | 1:39:B:THR:HG23 | 1:40:B:GLU:HA   | 15       | 0.48          |
| (1,1005) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HA   | 20       | 0.48          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 2        | 0.48          |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2  | 19       | 0.47          |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 17       | 0.47          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 13       | 0.47          |
| (1,3105) | 1:15:B:PHE:HE1  | 1:70:B:ASP:HB3  | 11       | 0.47          |
| (1,2517) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG3  | 16       | 0.47          |
| (1,2472) | 1:59:A:LYS:HG3  | 1:60:A:GLU:HB2  | 7        | 0.47          |
| (1,2100) | 1:25:A:LYS:HG3  | 1:26:A:TYR:HA   | 11       | 0.47          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 8        | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 8        | 0.47          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 8        | 0.47          |
| (1,1016) | 1:16:B:HIS:HE1  | 1:26:B:TYR:HD1  | 8        | 0.47          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 12       | 0.46          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 17       | 0.46          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 10       | 0.46          |
| (1,2329) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HB3  | 18       | 0.46          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 12       | 0.46          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 12       | 0.46          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 18       | 0.46          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 3        | 0.46          |
| (1,2949) | 1:15:B:PHE:HE2  | 1:19:B:SER:HA   | 7        | 0.45          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 7        | 0.45          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD21 | 18       | 0.45          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD22 | 18       | 0.45          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD23 | 18       | 0.45          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG2  | 6        | 0.45          |
| (1,1956) | 1:44:B:PHE:HD2  | 1:85:B:MET:HG3  | 6        | 0.45          |
| (1,1005) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HA   | 11       | 0.45          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 2        | 0.45          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 11       | 0.44          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 2        | 0.44          |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2  | 4        | 0.43          |
| (1,3484) | 1:57:A:VAL:H    | 1:58:A:MET:HG2  | 4        | 0.43          |
| (1,3484) | 1:57:A:VAL:H    | 1:58:A:MET:HG2  | 18       | 0.43          |
| (1,3177) | 1:27:A:LYS:HE3  | 1:71:A:PHE:H    | 12       | 0.43          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 4        | 0.43          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 5        | 0.43          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 12       | 0.43          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 16       | 0.43          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 19       | 0.43          |
| (1,2321) | 1:25:A:LYS:HA   | 1:26:A:TYR:HD1  | 5        | 0.43          |
| (1,1833) | 1:25:A:LYS:HB2  | 1:26:A:TYR:HE1  | 9        | 0.43          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 2        | 0.43          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 2        | 0.43          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 2        | 0.43          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 12       | 0.43          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 18       | 0.43          |
| (1,3539) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB3  | 11       | 0.42          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 14       | 0.42          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 2        | 0.42          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 3        | 0.42          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG  | 6        | 0.42          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG  | 17       | 0.42          |
| (1,2205) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB2 | 19       | 0.42          |
| (1,2035) | 1:15:B:PHE:HD1  | 1:28:B:LEU:HB3 | 18       | 0.42          |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1 | 6        | 0.42          |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1 | 6        | 0.42          |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1 | 6        | 0.42          |
| (1,1616) | 1:30:A:LYS:HE2  | 1:33:A:LEU:HB3 | 13       | 0.42          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2 | 13       | 0.42          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1 | 3        | 0.42          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2 | 3        | 0.42          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3 | 3        | 0.42          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA  | 18       | 0.42          |
| (1,856)  | 1:89:B:PHE:HB3  | 1:90:B:TRP:HD1 | 18       | 0.42          |
| (1,210)  | 1:91:A:GLU:HG3  | 1:26:B:TYR:HE1 | 1        | 0.42          |
| (1,209)  | 1:91:A:GLU:HG2  | 1:26:B:TYR:HE1 | 8        | 0.42          |
| (1,39)   | 1:4:A:LEU:HD21  | 1:40:B:GLU:HA  | 19       | 0.42          |
| (1,39)   | 1:4:A:LEU:HD22  | 1:40:B:GLU:HA  | 19       | 0.42          |
| (1,39)   | 1:4:A:LEU:HD23  | 1:40:B:GLU:HA  | 19       | 0.42          |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2 | 14       | 0.41          |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H   | 15       | 0.41          |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2 | 6        | 0.41          |
| (1,3484) | 1:57:A:VAL:H    | 1:58:A:MET:HG2 | 9        | 0.41          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG  | 1        | 0.41          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG  | 13       | 0.41          |
| (1,2205) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB2 | 2        | 0.41          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2 | 5        | 0.41          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2 | 6        | 0.41          |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2 | 13       | 0.41          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H   | 19       | 0.4           |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2 | 5        | 0.4           |
| (1,2472) | 1:59:A:LYS:HG3  | 1:60:A:GLU:HB2 | 1        | 0.4           |
| (1,2205) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB2 | 18       | 0.4           |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1 | 7        | 0.4           |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1 | 7        | 0.4           |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1 | 7        | 0.4           |
| (1,1831) | 1:41:B:LEU:HD11 | 1:44:B:PHE:HD1 | 16       | 0.4           |
| (1,1831) | 1:41:B:LEU:HD12 | 1:44:B:PHE:HD1 | 16       | 0.4           |
| (1,1831) | 1:41:B:LEU:HD13 | 1:44:B:PHE:HD1 | 16       | 0.4           |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2 | 11       | 0.4           |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1 | 4        | 0.4           |
| (1,1001) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HA  | 17       | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 4        | 0.4           |
| (1,511)  | 1:44:A:PHE:HA   | 1:44:A:PHE:HD2  | 7        | 0.4           |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2  | 13       | 0.39          |
| (1,3382) | 1:37:A:LEU:HA   | 1:40:A:GLU:HG3  | 1        | 0.39          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 9        | 0.39          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 18       | 0.39          |
| (1,2331) | 1:25:B:LYS:HA   | 1:26:B:TYR:HD1  | 8        | 0.39          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 14       | 0.39          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 14       | 0.39          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 14       | 0.39          |
| (1,538)  | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 3        | 0.39          |
| (1,538)  | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 3        | 0.39          |
| (1,538)  | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 3        | 0.39          |
| (1,522)  | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 3        | 0.39          |
| (1,522)  | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 3        | 0.39          |
| (1,3612) | 1:57:B:VAL:H    | 1:58:B:MET:HG2  | 8        | 0.38          |
| (1,3484) | 1:57:A:VAL:H    | 1:58:A:MET:HG2  | 19       | 0.38          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 17       | 0.38          |
| (1,3097) | 1:44:B:PHE:HE2  | 1:85:B:MET:H    | 9        | 0.38          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 8        | 0.38          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 20       | 0.38          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD21 | 17       | 0.38          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD22 | 17       | 0.38          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD23 | 17       | 0.38          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG21 | 19       | 0.38          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG22 | 19       | 0.38          |
| (1,1695) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG23 | 19       | 0.38          |
| (1,1616) | 1:30:A:LYS:HE2  | 1:33:A:LEU:HB3  | 2        | 0.38          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2  | 7        | 0.38          |
| (1,1349) | 1:39:A:THR:HG21 | 1:40:A:GLU:HA   | 2        | 0.38          |
| (1,1349) | 1:39:A:THR:HG22 | 1:40:A:GLU:HA   | 2        | 0.38          |
| (1,1349) | 1:39:A:THR:HG23 | 1:40:A:GLU:HA   | 2        | 0.38          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 3        | 0.38          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 3        | 0.38          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 3        | 0.38          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 18       | 0.37          |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 4        | 0.37          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 2        | 0.37          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 14       | 0.37          |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 19       | 0.36          |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 12       | 0.36          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 7        | 0.36          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3484) | 1:57:A:VAL:H   | 1:58:A:MET:HG2  | 15       | 0.36          |
| (1,3278) | 1:90:A:TRP:HE1 | 1:91:A:GLU:H    | 10       | 0.36          |
| (1,2824) | 1:44:A:PHE:H   | 1:45:A:LEU:HG   | 15       | 0.36          |
| (1,2528) | 1:15:B:PHE:HE1 | 1:74:B:TYR:HB3  | 20       | 0.36          |
| (1,2107) | 1:25:B:LYS:HG3 | 1:26:B:TYR:HA   | 17       | 0.36          |
| (1,2080) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD21 | 17       | 0.36          |
| (1,2080) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD22 | 17       | 0.36          |
| (1,2080) | 1:15:B:PHE:HD1 | 1:36:B:LEU:HD23 | 17       | 0.36          |
| (1,1684) | 1:55:B:ASP:HB3 | 1:56:B:LYS:HD2  | 14       | 0.36          |
| (1,210)  | 1:91:A:GLU:HG3 | 1:26:B:TYR:HE1  | 2        | 0.36          |
| (1,210)  | 1:91:A:GLU:HG3 | 1:26:B:TYR:HE1  | 11       | 0.36          |
| (1,3615) | 1:58:B:MET:HG2 | 1:59:B:LYS:HB2  | 1        | 0.35          |
| (1,3571) | 1:33:B:LEU:HB3 | 1:36:B:LEU:HG   | 10       | 0.35          |
| (1,3554) | 1:27:B:LYS:HB3 | 1:70:B:ASP:HB3  | 13       | 0.35          |
| (1,3521) | 1:1:B:GLY:HA2  | 1:5:B:GLU:HG2   | 11       | 0.35          |
| (1,3443) | 1:33:A:LEU:HB3 | 1:36:A:LEU:HG   | 10       | 0.35          |
| (1,3440) | 1:31:A:LYS:HE2 | 1:32:A:GLU:HG2  | 11       | 0.35          |
| (1,3420) | 1:19:A:SER:HB3 | 1:25:A:LYS:HB2  | 4        | 0.35          |
| (1,3282) | 1:90:B:TRP:HE1 | 1:91:B:GLU:H    | 3        | 0.35          |
| (1,3282) | 1:90:B:TRP:HE1 | 1:91:B:GLU:H    | 10       | 0.35          |
| (1,3105) | 1:15:B:PHE:HE1 | 1:70:B:ASP:HB3  | 19       | 0.35          |
| (1,2472) | 1:59:A:LYS:HG3 | 1:60:A:GLU:HB2  | 8        | 0.35          |
| (1,2148) | 1:25:B:LYS:HE3 | 1:26:B:TYR:HD1  | 11       | 0.35          |
| (1,1952) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG11 | 19       | 0.35          |
| (1,1952) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG12 | 19       | 0.35          |
| (1,1952) | 1:15:B:PHE:HE1 | 1:69:B:VAL:HG13 | 19       | 0.35          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE1  | 9        | 0.35          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE2  | 9        | 0.35          |
| (1,1144) | 1:44:A:PHE:HE2 | 1:85:A:MET:HE3  | 9        | 0.35          |
| (1,946)  | 1:25:B:LYS:HB2 | 1:26:B:TYR:HD1  | 8        | 0.35          |
| (1,892)  | 1:44:B:PHE:HE2 | 1:82:B:THR:HA   | 10       | 0.35          |
| (1,3619) | 1:64:B:ASN:HB3 | 1:67:B:GLY:H    | 17       | 0.34          |
| (1,3604) | 1:51:B:VAL:H   | 1:55:B:ASP:H    | 10       | 0.34          |
| (1,3604) | 1:51:B:VAL:H   | 1:55:B:ASP:H    | 17       | 0.34          |
| (1,3516) | 1:89:A:PHE:H   | 1:89:A:PHE:HE2  | 11       | 0.34          |
| (1,3282) | 1:90:B:TRP:HE1 | 1:91:B:GLU:H    | 8        | 0.34          |
| (1,3278) | 1:90:A:TRP:HE1 | 1:91:A:GLU:H    | 5        | 0.34          |
| (1,2987) | 1:25:A:LYS:HG2 | 1:26:A:TYR:HA   | 3        | 0.34          |
| (1,2321) | 1:25:A:LYS:HA  | 1:26:A:TYR:HD1  | 4        | 0.34          |
| (1,1452) | 1:22:A:GLU:HB2 | 1:31:A:LYS:HG2  | 17       | 0.34          |
| (1,1222) | 1:46:A:ASP:HA  | 1:49:A:LYS:HB2  | 13       | 0.34          |
| (1,1100) | 1:44:A:PHE:HD2 | 1:85:A:MET:HE1  | 3        | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 3        | 0.34          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 3        | 0.34          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 5        | 0.34          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 16       | 0.34          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 11       | 0.33          |
| (1,3477) | 1:51:A:VAL:HB   | 1:52:A:ASP:HB3  | 15       | 0.33          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 2        | 0.33          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 1        | 0.33          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 20       | 0.33          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 14       | 0.33          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 3        | 0.33          |
| (1,2520) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG3  | 19       | 0.33          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD21 | 12       | 0.33          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD22 | 12       | 0.33          |
| (1,2073) | 1:15:A:PHE:HD1  | 1:36:A:LEU:HD23 | 12       | 0.33          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD21  | 18       | 0.33          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD22  | 18       | 0.33          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD23  | 18       | 0.33          |
| (1,1623) | 1:30:B:LYS:HE2  | 1:33:B:LEU:HB3  | 17       | 0.33          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 7        | 0.33          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 7        | 0.33          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 7        | 0.33          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 13       | 0.33          |
| (1,165)  | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 4        | 0.33          |
| (1,165)  | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 4        | 0.33          |
| (1,165)  | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 4        | 0.33          |
| (1,3615) | 1:58:B:MET:HG2  | 1:59:B:LYS:HB2  | 10       | 0.32          |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 3        | 0.32          |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 8        | 0.32          |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 11       | 0.32          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 15       | 0.32          |
| (1,3411) | 1:15:A:PHE:HE2  | 1:27:A:LYS:HB3  | 17       | 0.32          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 1        | 0.32          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 15       | 0.32          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 19       | 0.32          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 18       | 0.32          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 1        | 0.32          |
| (1,2824) | 1:44:A:PHE:H    | 1:45:A:LEU:HG   | 14       | 0.32          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 3        | 0.32          |
| (1,888)  | 1:44:A:PHE:HE2  | 1:82:A:THR:HA   | 5        | 0.32          |
| (1,203)  | 1:90:A:TRP:HB2  | 1:26:B:TYR:HE1  | 1        | 0.32          |
| (1,203)  | 1:90:A:TRP:HB2  | 1:26:B:TYR:HE1  | 15       | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3550) | 1:22:B:GLU:HB2  | 1:29:B:SER:HA   | 4        | 0.31          |
| (1,3516) | 1:89:A:PHE:H    | 1:89:A:PHE:HE2  | 19       | 0.31          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 1        | 0.31          |
| (1,3231) | 1:75:B:VAL:H    | 1:76:B:VAL:HB   | 20       | 0.31          |
| (1,3227) | 1:75:A:VAL:H    | 1:76:A:VAL:HB   | 6        | 0.31          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 20       | 0.31          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 3        | 0.31          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 14       | 0.31          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 20       | 0.31          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 12       | 0.31          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 12       | 0.31          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 12       | 0.31          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 5        | 0.31          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 5        | 0.31          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 5        | 0.31          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 9        | 0.3           |
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 9        | 0.3           |
| (1,3597) | 1:48:B:GLN:HE21 | 1:50:B:ASP:H    | 10       | 0.3           |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 12       | 0.3           |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 14       | 0.3           |
| (1,3470) | 1:48:A:GLN:HE22 | 1:49:A:LYS:H    | 4        | 0.3           |
| (1,3294) | 1:59:A:LYS:H    | 1:61:A:LEU:HD21 | 2        | 0.3           |
| (1,3294) | 1:59:A:LYS:H    | 1:61:A:LEU:HD22 | 2        | 0.3           |
| (1,3294) | 1:59:A:LYS:H    | 1:61:A:LEU:HD23 | 2        | 0.3           |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 9        | 0.3           |
| (1,3275) | 1:26:A:TYR:HA   | 1:27:A:LYS:HD2  | 14       | 0.3           |
| (1,2991) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HA   | 5        | 0.3           |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 8        | 0.3           |
| (1,2612) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HD3  | 4        | 0.3           |
| (1,2148) | 1:25:B:LYS:HE3  | 1:26:B:TYR:HD1  | 10       | 0.3           |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD21  | 17       | 0.3           |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD22  | 17       | 0.3           |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD23  | 17       | 0.3           |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 7        | 0.3           |
| (1,869)  | 1:11:B:LEU:HA   | 1:14:B:VAL:HB   | 9        | 0.3           |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 2        | 0.3           |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 3        | 0.3           |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 3        | 0.3           |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 3        | 0.3           |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 20       | 0.3           |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 20       | 0.3           |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 20       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 20       | 0.3           |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 20       | 0.3           |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 20       | 0.3           |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 20       | 0.3           |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 20       | 0.3           |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 20       | 0.3           |
| (1,201)  | 1:42:A:SER:H    | 1:1:B:GLY:HA2   | 13       | 0.3           |
| (1,201)  | 1:42:A:SER:H    | 1:1:B:GLY:HA3   | 13       | 0.3           |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 7        | 0.29          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 2        | 0.29          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 16       | 0.29          |
| (1,3231) | 1:75:B:VAL:H    | 1:76:B:VAL:HB   | 13       | 0.29          |
| (1,3231) | 1:75:B:VAL:H    | 1:76:B:VAL:HB   | 16       | 0.29          |
| (1,2991) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HA   | 15       | 0.29          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 11       | 0.29          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 12       | 0.29          |
| (1,2329) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HB3  | 17       | 0.29          |
| (1,2107) | 1:25:B:LYS:HG3  | 1:26:B:TYR:HA   | 12       | 0.29          |
| (1,2103) | 1:63:A:GLU:HB2  | 1:64:A:ASN:HD21 | 6        | 0.29          |
| (1,2100) | 1:25:A:LYS:HG3  | 1:26:A:TYR:HA   | 19       | 0.29          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG11 | 17       | 0.29          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG12 | 17       | 0.29          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG13 | 17       | 0.29          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 19       | 0.29          |
| (1,1530) | 1:24:A:ASP:HB2  | 1:27:A:LYS:HG2  | 18       | 0.29          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2  | 2        | 0.29          |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 5        | 0.29          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 3        | 0.29          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 3        | 0.29          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 3        | 0.29          |
| (1,927)  | 1:21:B:LYS:HA   | 1:21:B:LYS:HE2  | 17       | 0.29          |
| (1,665)  | 1:39:A:THR:HG21 | 1:40:A:GLU:HG2  | 20       | 0.29          |
| (1,665)  | 1:39:A:THR:HG22 | 1:40:A:GLU:HG2  | 20       | 0.29          |
| (1,665)  | 1:39:A:THR:HG23 | 1:40:A:GLU:HG2  | 20       | 0.29          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 14       | 0.29          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 19       | 0.29          |
| (1,522)  | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 12       | 0.29          |
| (1,522)  | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 12       | 0.29          |
| (1,515)  | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 7        | 0.29          |
| (1,254)  | 1:89:A:PHE:HD2  | 1:9:B:GLU:HG2   | 20       | 0.29          |
| (1,3615) | 1:58:B:MET:HG2  | 1:59:B:LYS:HB2  | 3        | 0.28          |
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 5        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 12       | 0.28          |
| (1,3564) | 1:29:B:SER:HA   | 1:31:B:LYS:HE3  | 7        | 0.28          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 6        | 0.28          |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 3        | 0.28          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 10       | 0.28          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 10       | 0.28          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 10       | 0.28          |
| (1,3424) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HE1  | 17       | 0.28          |
| (1,3422) | 1:22:A:GLU:HB2  | 1:29:A:SER:HA   | 13       | 0.28          |
| (1,2987) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HA   | 19       | 0.28          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 19       | 0.28          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG11 | 17       | 0.28          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG12 | 17       | 0.28          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG13 | 17       | 0.28          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 8        | 0.28          |
| (1,1616) | 1:30:A:LYS:HE2  | 1:33:A:LEU:HB3  | 20       | 0.28          |
| (1,1395) | 1:31:B:LYS:HB2  | 1:32:B:GLU:H    | 20       | 0.28          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1  | 5        | 0.28          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2  | 5        | 0.28          |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3  | 5        | 0.28          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 12       | 0.28          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 12       | 0.28          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 12       | 0.28          |
| (1,1016) | 1:16:B:HIS:HE1  | 1:26:B:TYR:HD1  | 15       | 0.28          |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 13       | 0.28          |
| (1,659)  | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG21 | 12       | 0.28          |
| (1,659)  | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG22 | 12       | 0.28          |
| (1,659)  | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG23 | 12       | 0.28          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 13       | 0.28          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 6        | 0.28          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 3        | 0.28          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 8        | 0.28          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 8        | 0.28          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 8        | 0.28          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 13       | 0.27          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 15       | 0.27          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 8        | 0.27          |
| (1,3550) | 1:22:B:GLU:HB2  | 1:29:B:SER:HA   | 1        | 0.27          |
| (1,3436) | 1:29:A:SER:HA   | 1:31:A:LYS:HE3  | 4        | 0.27          |
| (1,3312) | 1:45:B:LEU:HA   | 1:49:B:LYS:HG2  | 12       | 0.27          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 4        | 0.27          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 8        | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 6        | 0.27          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 4        | 0.27          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 13       | 0.27          |
| (1,3227) | 1:75:A:VAL:H    | 1:76:A:VAL:HB   | 20       | 0.27          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 9        | 0.27          |
| (1,2319) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HB3  | 7        | 0.27          |
| (1,2319) | 1:15:A:PHE:HD1  | 1:74:A:TYR:HB3  | 18       | 0.27          |
| (1,2205) | 1:15:B:PHE:HE1  | 1:74:B:TYR:HB2  | 11       | 0.27          |
| (1,2107) | 1:25:B:LYS:HG3  | 1:26:B:TYR:HA   | 15       | 0.27          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD21  | 15       | 0.27          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD22  | 15       | 0.27          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD23  | 15       | 0.27          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 5        | 0.27          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 16       | 0.27          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD21  | 8        | 0.27          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD22  | 8        | 0.27          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD23  | 8        | 0.27          |
| (1,1565) | 1:22:B:GLU:HB3  | 1:31:B:LYS:HD2  | 20       | 0.27          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 4        | 0.27          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 4        | 0.27          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 4        | 0.27          |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 20       | 0.27          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE1  | 10       | 0.27          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE2  | 10       | 0.27          |
| (1,1100) | 1:44:A:PHE:HD2  | 1:85:A:MET:HE3  | 10       | 0.27          |
| (1,892)  | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 3        | 0.27          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 8        | 0.27          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 1        | 0.27          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 12       | 0.27          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 17       | 0.27          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 14       | 0.27          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 14       | 0.27          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 14       | 0.27          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 19       | 0.27          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 19       | 0.27          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 19       | 0.27          |
| (1,386)  | 1:30:A:LYS:HG3  | 1:65:A:GLY:HA3  | 11       | 0.27          |
| (1,348)  | 1:12:B:ILE:HG21 | 1:16:B:HIS:HD2  | 13       | 0.27          |
| (1,348)  | 1:12:B:ILE:HG22 | 1:16:B:HIS:HD2  | 13       | 0.27          |
| (1,348)  | 1:12:B:ILE:HG23 | 1:16:B:HIS:HD2  | 13       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 19       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 19       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 19       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 19       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 19       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 19       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 19       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 19       | 0.27          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 19       | 0.27          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 16       | 0.27          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 16       | 0.27          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 16       | 0.27          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 4        | 0.26          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 6        | 0.26          |
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 13       | 0.26          |
| (1,3519) | 1:91:A:GLU:HB2  | 1:93:A:SER:H    | 3        | 0.26          |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 6        | 0.26          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 11       | 0.26          |
| (1,3489) | 1:63:A:GLU:HA   | 1:66:A:ASP:HB2  | 10       | 0.26          |
| (1,3489) | 1:63:A:GLU:HA   | 1:66:A:ASP:HB2  | 14       | 0.26          |
| (1,3457) | 1:43:A:GLY:H    | 1:46:A:ASP:HB3  | 14       | 0.26          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 6        | 0.26          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 6        | 0.26          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 6        | 0.26          |
| (1,3373) | 1:13:B:ASN:H    | 1:16:B:HIS:HD2  | 11       | 0.26          |
| (1,3308) | 1:45:A:LEU:HA   | 1:49:A:LYS:HG2  | 17       | 0.26          |
| (1,3279) | 1:26:B:TYR:HA   | 1:27:B:LYS:HD2  | 17       | 0.26          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 3        | 0.26          |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 6        | 0.26          |
| (1,3101) | 1:15:A:PHE:HE1  | 1:70:A:ASP:HB3  | 7        | 0.26          |
| (1,2987) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HA   | 17       | 0.26          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 13       | 0.26          |
| (1,2612) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HD3  | 18       | 0.26          |
| (1,2329) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HB3  | 11       | 0.26          |
| (1,2110) | 1:63:B:GLU:HB2  | 1:64:B:ASN:HD21 | 17       | 0.26          |
| (1,2100) | 1:25:A:LYS:HG3  | 1:26:A:TYR:HA   | 17       | 0.26          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 20       | 0.26          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 12       | 0.26          |
| (1,1565) | 1:22:B:GLU:HB3  | 1:31:B:LYS:HD2  | 16       | 0.26          |
| (1,1395) | 1:31:B:LYS:HB2  | 1:32:B:GLU:H    | 9        | 0.26          |
| (1,1034) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HA   | 17       | 0.26          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 1        | 0.26          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 1        | 0.26          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 1        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 4        | 0.26          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 4        | 0.26          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 4        | 0.26          |
| (1,927)  | 1:21:B:LYS:HA   | 1:21:B:LYS:HE2  | 15       | 0.26          |
| (1,856)  | 1:89:B:PHE:HB3  | 1:90:B:TRP:HD1  | 12       | 0.26          |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 16       | 0.26          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 16       | 0.26          |
| (1,479)  | 1:89:A:PHE:HA   | 1:89:A:PHE:HD1  | 15       | 0.26          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 4        | 0.26          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 4        | 0.26          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 4        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 6        | 0.26          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 13       | 0.26          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 13       | 0.26          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 17       | 0.26          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 17       | 0.26          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 17       | 0.26          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 18       | 0.26          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 18       | 0.26          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 18       | 0.26          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 17       | 0.26          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 17       | 0.26          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 17       | 0.26          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 13       | 0.25          |
| (1,3615) | 1:58:B:MET:HG2  | 1:59:B:LYS:HB2  | 18       | 0.25          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 10       | 0.25          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 10       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 10       | 0.25          |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 7        | 0.25          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 3        | 0.25          |
| (1,3539) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HB3  | 20       | 0.25          |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 8        | 0.25          |
| (1,3476) | 1:51:A:VAL:H    | 1:55:A:ASP:H    | 4        | 0.25          |
| (1,3476) | 1:51:A:VAL:H    | 1:55:A:ASP:H    | 17       | 0.25          |
| (1,3470) | 1:48:A:GLN:HE22 | 1:49:A:LYS:H    | 6        | 0.25          |
| (1,3279) | 1:26:B:TYR:HA   | 1:27:B:LYS:HD2  | 18       | 0.25          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 15       | 0.25          |
| (1,3275) | 1:26:A:TYR:HA   | 1:27:A:LYS:HD2  | 6        | 0.25          |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 18       | 0.25          |
| (1,3133) | 1:57:A:VAL:H    | 1:58:A:MET:HB3  | 2        | 0.25          |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 13       | 0.25          |
| (1,2991) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HA   | 19       | 0.25          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 12       | 0.25          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 10       | 0.25          |
| (1,2601) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HD3  | 5        | 0.25          |
| (1,2601) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HD3  | 13       | 0.25          |
| (1,2472) | 1:59:A:LYS:HG3  | 1:60:A:GLU:HB2  | 15       | 0.25          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 12       | 0.25          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 2        | 0.25          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 6        | 0.25          |
| (1,2107) | 1:25:B:LYS:HG3  | 1:26:B:TYR:HA   | 5        | 0.25          |
| (1,2107) | 1:25:B:LYS:HG3  | 1:26:B:TYR:HA   | 19       | 0.25          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG11 | 11       | 0.25          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG12 | 11       | 0.25          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG13 | 11       | 0.25          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG11 | 12       | 0.25          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG12 | 12       | 0.25          |
| (1,1940) | 1:15:A:PHE:HE1  | 1:69:A:VAL:HG13 | 12       | 0.25          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 3        | 0.25          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 8        | 0.25          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 12       | 0.25          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 1        | 0.25          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2  | 15       | 0.25          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 9        | 0.25          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 9        | 0.25          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 9        | 0.25          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 19       | 0.25          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 19       | 0.25          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 19       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,963)  | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 9        | 0.25          |
| (1,927)  | 1:21:B:LYS:HA   | 1:21:B:LYS:HE2  | 7        | 0.25          |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 12       | 0.25          |
| (1,694)  | 1:59:B:LYS:HA   | 1:59:B:LYS:HE2  | 9        | 0.25          |
| (1,694)  | 1:59:B:LYS:HA   | 1:59:B:LYS:HE3  | 9        | 0.25          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 10       | 0.25          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 19       | 0.25          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 11       | 0.25          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 11       | 0.25          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 11       | 0.25          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 8        | 0.25          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 8        | 0.25          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 8        | 0.25          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 7        | 0.25          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 13       | 0.25          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 16       | 0.25          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 20       | 0.25          |
| (1,395)  | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 15       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 12       | 0.25          |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 12       | 0.25          |
| (1,144)  | 1:11:A:LEU:HD11 | 1:4:B:LEU:HB2   | 17       | 0.25          |
| (1,144)  | 1:11:A:LEU:HD12 | 1:4:B:LEU:HB2   | 17       | 0.25          |
| (1,144)  | 1:11:A:LEU:HD13 | 1:4:B:LEU:HB2   | 17       | 0.25          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 3        | 0.25          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 3        | 0.25          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 3        | 0.25          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 15       | 0.25          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 15       | 0.25          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 15       | 0.25          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 12       | 0.25          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 12       | 0.25          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 12       | 0.25          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 11       | 0.24          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 12       | 0.24          |
| (1,3615) | 1:58:B:MET:HG2  | 1:59:B:LYS:HB2  | 2        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 14       | 0.24          |
| (1,3549) | 1:20:B:GLY:HA3  | 1:21:B:LYS:HE2  | 15       | 0.24          |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 18       | 0.24          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 8        | 0.24          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 13       | 0.24          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 13       | 0.24          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 13       | 0.24          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 1        | 0.24          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 4        | 0.24          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 1        | 0.24          |
| (1,3422) | 1:22:A:GLU:HB2  | 1:29:A:SER:HA   | 7        | 0.24          |
| (1,3385) | 1:66:A:ASP:HB2  | 1:68:A:GLU:H    | 17       | 0.24          |
| (1,3312) | 1:45:B:LEU:HA   | 1:49:B:LYS:HG2  | 20       | 0.24          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 11       | 0.24          |
| (1,3279) | 1:26:B:TYR:HA   | 1:27:B:LYS:HD2  | 9        | 0.24          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 6        | 0.24          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 11       | 0.24          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 13       | 0.24          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 14       | 0.24          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 15       | 0.24          |
| (1,2991) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HA   | 17       | 0.24          |
| (1,2987) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HA   | 2        | 0.24          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 9        | 0.24          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 1        | 0.24          |
| (1,2354) | 1:21:B:LYS:HG3  | 1:32:B:GLU:HB3  | 8        | 0.24          |
| (1,2110) | 1:63:B:GLU:HB2  | 1:64:B:ASN:HD21 | 5        | 0.24          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD21 | 7        | 0.24          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD22 | 7        | 0.24          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD23 | 7        | 0.24          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 13       | 0.24          |
| (1,1593) | 1:25:B:LYS:HB2  | 1:25:B:LYS:HE3  | 10       | 0.24          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE1  | 2        | 0.24          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE2  | 2        | 0.24          |
| (1,1148) | 1:44:B:PHE:HE2  | 1:85:B:MET:HE3  | 2        | 0.24          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1  | 16       | 0.24          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2  | 16       | 0.24          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3  | 16       | 0.24          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 1        | 0.24          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 1        | 0.24          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 1        | 0.24          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 9        | 0.24          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 9        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 9        | 0.24          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 16       | 0.24          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 16       | 0.24          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 16       | 0.24          |
| (1,856)  | 1:89:B:PHE:HB3  | 1:90:B:TRP:HD1  | 2        | 0.24          |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 11       | 0.24          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 10       | 0.24          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 2        | 0.24          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 20       | 0.24          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 16       | 0.24          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 16       | 0.24          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 16       | 0.24          |
| (1,457)  | 1:30:B:LYS:HD3  | 1:65:B:GLY:HA2  | 17       | 0.24          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 16       | 0.24          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 16       | 0.24          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 16       | 0.24          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 10       | 0.24          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 10       | 0.24          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 10       | 0.24          |
| (1,395)  | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 19       | 0.24          |
| (1,390)  | 1:30:B:LYS:HG3  | 1:65:B:GLY:HA3  | 9        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 7        | 0.24          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 7        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 8        | 0.24          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 8        | 0.24          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 12       | 0.24          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 12       | 0.24          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 12       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 14       | 0.24          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 14       | 0.24          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 14       | 0.24          |
| (1,3620) | 1:68:B:GLU:HB3  | 1:70:B:ASP:HB3  | 4        | 0.23          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 1        | 0.23          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 7        | 0.23          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 11       | 0.23          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 11       | 0.23          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 11       | 0.23          |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 11       | 0.23          |
| (1,3489) | 1:63:A:GLU:HA   | 1:66:A:ASP:HB2  | 19       | 0.23          |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 13       | 0.23          |
| (1,3476) | 1:51:A:VAL:H    | 1:55:A:ASP:H    | 9        | 0.23          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 3        | 0.23          |
| (1,3422) | 1:22:A:GLU:HB2  | 1:29:A:SER:HA   | 17       | 0.23          |
| (1,3275) | 1:26:A:TYR:HA   | 1:27:A:LYS:HD2  | 12       | 0.23          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 3        | 0.23          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 19       | 0.23          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 14       | 0.23          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 3        | 0.23          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 17       | 0.23          |
| (1,2571) | 1:31:B:LYS:HG3  | 1:32:B:GLU:HG3  | 13       | 0.23          |
| (1,2563) | 1:31:A:LYS:HG3  | 1:32:A:GLU:HG3  | 9        | 0.23          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 5        | 0.23          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 16       | 0.23          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 17       | 0.23          |
| (1,2354) | 1:21:B:LYS:HG3  | 1:32:B:GLU:HB3  | 20       | 0.23          |
| (1,2189) | 1:29:B:SER:HA   | 1:31:B:LYS:HE2  | 2        | 0.23          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 3        | 0.23          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 3        | 0.23          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 3        | 0.23          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 17       | 0.23          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 17       | 0.23          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 17       | 0.23          |
| (1,2103) | 1:63:A:GLU:HB2  | 1:64:A:ASN:HD21 | 4        | 0.23          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 5        | 0.23          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 4        | 0.23          |
| (1,1623) | 1:30:B:LYS:HE2  | 1:33:B:LEU:HB3  | 14       | 0.23          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 5        | 0.23          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 5        | 0.23          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 5        | 0.23          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 6        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 6        | 0.23          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 6        | 0.23          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 14       | 0.23          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 14       | 0.23          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 14       | 0.23          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 18       | 0.23          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 18       | 0.23          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 18       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 19       | 0.23          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 19       | 0.23          |
| (1,967)  | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 1        | 0.23          |
| (1,967)  | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 1        | 0.23          |
| (1,967)  | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 1        | 0.23          |
| (1,613)  | 1:25:B:LYS:HG3  | 1:25:B:LYS:HE3  | 15       | 0.23          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 15       | 0.23          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 9        | 0.23          |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 11       | 0.23          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE2  | 11       | 0.23          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE3  | 11       | 0.23          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE2  | 13       | 0.23          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE3  | 13       | 0.23          |
| (1,454)  | 1:30:A:LYS:HD3  | 1:65:A:GLY:HA2  | 14       | 0.23          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 18       | 0.23          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 18       | 0.23          |
| (1,447)  | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 18       | 0.23          |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD11  | 17       | 0.23          |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD12  | 17       | 0.23          |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD13  | 17       | 0.23          |
| (1,437)  | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 1        | 0.23          |
| (1,437)  | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 1        | 0.23          |
| (1,437)  | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 1        | 0.23          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 4        | 0.23          |
| (1,395)  | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 1        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 8        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 8        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,328)  | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 8        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 8        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 8        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 8        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 8        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 8        | 0.23          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 8        | 0.23          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 12       | 0.23          |
| (1,327)  | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 12       | 0.23          |
| (1,277)  | 1:61:A:LEU:HA   | 1:61:A:LEU:HD11 | 2        | 0.23          |
| (1,277)  | 1:61:A:LEU:HA   | 1:61:A:LEU:HD12 | 2        | 0.23          |
| (1,277)  | 1:61:A:LEU:HA   | 1:61:A:LEU:HD13 | 2        | 0.23          |
| (1,248)  | 1:87:A:ASN:HA   | 1:12:B:ILE:HD11 | 4        | 0.23          |
| (1,248)  | 1:87:A:ASN:HA   | 1:12:B:ILE:HD12 | 4        | 0.23          |
| (1,248)  | 1:87:A:ASN:HA   | 1:12:B:ILE:HD13 | 4        | 0.23          |
| (1,167)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HG2  | 3        | 0.23          |
| (1,167)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HG2  | 3        | 0.23          |
| (1,167)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HG2  | 3        | 0.23          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 7        | 0.23          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 7        | 0.23          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 7        | 0.23          |
| (1,81)   | 1:72:A:GLN:HA   | 1:80:B:ALA:HA   | 16       | 0.23          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 6        | 0.22          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 6        | 0.22          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 12       | 0.22          |
| (1,3598) | 1:48:B:GLN:HE22 | 1:49:B:LYS:H    | 4        | 0.22          |
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 9        | 0.22          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 3        | 0.22          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 6        | 0.22          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 12       | 0.22          |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 2        | 0.22          |
| (1,3421) | 1:20:A:GLY:HA3  | 1:21:A:LYS:HE2  | 9        | 0.22          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 19       | 0.22          |
| (1,3400) | 1:9:A:GLU:HA    | 1:71:A:PHE:HE2  | 20       | 0.22          |
| (1,3394) | 1:6:A:THR:HG21  | 1:9:A:GLU:HA    | 1        | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3394) | 1:6:A:THR:HG22  | 1:9:A:GLU:HA    | 1        | 0.22          |
| (1,3394) | 1:6:A:THR:HG23  | 1:9:A:GLU:HA    | 1        | 0.22          |
| (1,3394) | 1:6:A:THR:HG21  | 1:9:A:GLU:HA    | 14       | 0.22          |
| (1,3394) | 1:6:A:THR:HG22  | 1:9:A:GLU:HA    | 14       | 0.22          |
| (1,3394) | 1:6:A:THR:HG23  | 1:9:A:GLU:HA    | 14       | 0.22          |
| (1,3385) | 1:66:A:ASP:HB2  | 1:68:A:GLU:H    | 7        | 0.22          |
| (1,3275) | 1:26:A:TYR:HA   | 1:27:A:LYS:HD2  | 7        | 0.22          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 5        | 0.22          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 6        | 0.22          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 9        | 0.22          |
| (1,3034) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HE1  | 7        | 0.22          |
| (1,3034) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HE1  | 7        | 0.22          |
| (1,3034) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HE1  | 7        | 0.22          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 12       | 0.22          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 17       | 0.22          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 15       | 0.22          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 17       | 0.22          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 19       | 0.22          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 3        | 0.22          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 12       | 0.22          |
| (1,2401) | 1:1:B:GLY:HA2   | 1:5:B:GLU:HB3   | 12       | 0.22          |
| (1,2329) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HB3  | 19       | 0.22          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG11 | 2        | 0.22          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG12 | 2        | 0.22          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG13 | 2        | 0.22          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 1        | 0.22          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 6        | 0.22          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 6        | 0.22          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 6        | 0.22          |
| (1,1565) | 1:22:B:GLU:HB3  | 1:31:B:LYS:HD2  | 11       | 0.22          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 11       | 0.22          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 11       | 0.22          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 11       | 0.22          |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 4        | 0.22          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 19       | 0.22          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 19       | 0.22          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 19       | 0.22          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 19       | 0.22          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 19       | 0.22          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 19       | 0.22          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 19       | 0.22          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 19       | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 19       | 0.22          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 19       | 0.22          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 19       | 0.22          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 19       | 0.22          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 11       | 0.22          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 11       | 0.22          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 11       | 0.22          |
| (1,794) | 1:39:B:THR:H    | 1:39:B:THR:HG21 | 14       | 0.22          |
| (1,794) | 1:39:B:THR:H    | 1:39:B:THR:HG22 | 14       | 0.22          |
| (1,794) | 1:39:B:THR:H    | 1:39:B:THR:HG23 | 14       | 0.22          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 17       | 0.22          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 17       | 0.22          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 17       | 0.22          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 4        | 0.22          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 4        | 0.22          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 4        | 0.22          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 4        | 0.22          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 9        | 0.22          |
| (1,545) | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 3        | 0.22          |
| (1,545) | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 5        | 0.22          |
| (1,545) | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 8        | 0.22          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 11       | 0.22          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 11       | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 2        | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 2        | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 2        | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 6        | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 6        | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 6        | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 12       | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 12       | 0.22          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 12       | 0.22          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 11       | 0.22          |
| (1,339) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HD2  | 13       | 0.22          |
| (1,339) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HD2  | 13       | 0.22          |
| (1,339) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HD2  | 13       | 0.22          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 15       | 0.22          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 15       | 0.22          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 15       | 0.22          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 15       | 0.22          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 15       | 0.22          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 15       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 15       | 0.22          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 15       | 0.22          |
| (1,328)  | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 15       | 0.22          |
| (1,203)  | 1:90:A:TRP:HB2  | 1:26:B:TYR:HE1  | 2        | 0.22          |
| (1,176)  | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 2        | 0.22          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 11       | 0.22          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 11       | 0.22          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 11       | 0.22          |
| (1,165)  | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 13       | 0.22          |
| (1,165)  | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 13       | 0.22          |
| (1,165)  | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 13       | 0.22          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 10       | 0.22          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 16       | 0.22          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 14       | 0.22          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 14       | 0.22          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 14       | 0.22          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 20       | 0.22          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 20       | 0.22          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 20       | 0.22          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 20       | 0.21          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 8        | 0.21          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 14       | 0.21          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 20       | 0.21          |
| (1,3615) | 1:58:B:MET:HG2  | 1:59:B:LYS:HB2  | 11       | 0.21          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 16       | 0.21          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 16       | 0.21          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 16       | 0.21          |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 11       | 0.21          |
| (1,3550) | 1:22:B:GLU:HB2  | 1:29:B:SER:HA   | 18       | 0.21          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 12       | 0.21          |
| (1,3489) | 1:63:A:GLU:HA   | 1:66:A:ASP:HB2  | 17       | 0.21          |
| (1,3476) | 1:51:A:VAL:H    | 1:55:A:ASP:H    | 8        | 0.21          |
| (1,3470) | 1:48:A:GLN:HE22 | 1:49:A:LYS:H    | 19       | 0.21          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 11       | 0.21          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 11       | 0.21          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 11       | 0.21          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 5        | 0.21          |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 12       | 0.21          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 12       | 0.21          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 19       | 0.21          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 13       | 0.21          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 7        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 16       | 0.21          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 19       | 0.21          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 11       | 0.21          |
| (1,2329) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HB3  | 2        | 0.21          |
| (1,2198) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB2  | 12       | 0.21          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 2        | 0.21          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 2        | 0.21          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 2        | 0.21          |
| (1,2110) | 1:63:B:GLU:HB2  | 1:64:B:ASN:HD21 | 15       | 0.21          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 4        | 0.21          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 11       | 0.21          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 6        | 0.21          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 10       | 0.21          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 11       | 0.21          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 11       | 0.21          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 11       | 0.21          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 14       | 0.21          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 14       | 0.21          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 14       | 0.21          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 15       | 0.21          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 15       | 0.21          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 15       | 0.21          |
| (1,1395) | 1:31:B:LYS:HB2  | 1:32:B:GLU:H    | 11       | 0.21          |
| (1,1278) | 1:89:B:PHE:HB2  | 1:90:B:TRP:HD1  | 7        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 5        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 5        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 5        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 6        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 6        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 6        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 7        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 7        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 7        | 0.21          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 11       | 0.21          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 11       | 0.21          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 11       | 0.21          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 14       | 0.21          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 14       | 0.21          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 14       | 0.21          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 14       | 0.21          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 14       | 0.21          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 14       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 14       | 0.21          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 14       | 0.21          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 14       | 0.21          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD11 | 1        | 0.21          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD12 | 1        | 0.21          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD13 | 1        | 0.21          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 11       | 0.21          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 11       | 0.21          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 11       | 0.21          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 13       | 0.21          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 13       | 0.21          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 13       | 0.21          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 5        | 0.21          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 17       | 0.21          |
| (1,545) | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 4        | 0.21          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 20       | 0.21          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 20       | 0.21          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 20       | 0.21          |
| (1,499) | 1:57:A:VAL:HG21 | 1:81:A:LEU:HG   | 17       | 0.21          |
| (1,499) | 1:57:A:VAL:HG22 | 1:81:A:LEU:HG   | 17       | 0.21          |
| (1,499) | 1:57:A:VAL:HG23 | 1:81:A:LEU:HG   | 17       | 0.21          |
| (1,479) | 1:89:A:PHE:HA   | 1:89:A:PHE:HD1  | 19       | 0.21          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 14       | 0.21          |
| (1,386) | 1:30:A:LYS:HG3  | 1:65:A:GLY:HA3  | 4        | 0.21          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 1        | 0.21          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 1        | 0.21          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 4        | 0.21          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 4        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 20       | 0.21          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 20       | 0.21          |
| (1,267)  | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2  | 17       | 0.21          |
| (1,267)  | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2  | 17       | 0.21          |
| (1,267)  | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2  | 17       | 0.21          |
| (1,210)  | 1:91:A:GLU:HG3  | 1:26:B:TYR:HE1  | 15       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 10       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 10       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 10       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 13       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 13       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 13       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 15       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 15       | 0.21          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 15       | 0.21          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 5        | 0.21          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 4        | 0.21          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 4        | 0.21          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 4        | 0.21          |
| (1,3644) | 1:89:B:PHE:H    | 1:89:B:PHE:HE2  | 19       | 0.2           |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 4        | 0.2           |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 16       | 0.2           |
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 8        | 0.2           |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 1        | 0.2           |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 1        | 0.2           |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 1        | 0.2           |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 17       | 0.2           |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 6        | 0.2           |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 19       | 0.2           |
| (1,3550) | 1:22:B:GLU:HB2  | 1:29:B:SER:HA   | 2        | 0.2           |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 14       | 0.2           |
| (1,3492) | 1:68:A:GLU:HB3  | 1:70:A:ASP:HB3  | 20       | 0.2           |
| (1,3470) | 1:48:A:GLN:HE22 | 1:49:A:LYS:H    | 5        | 0.2           |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 15       | 0.2           |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 15       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 15       | 0.2           |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 8        | 0.2           |
| (1,3367) | 1:13:A:ASN:H    | 1:16:A:HIS:HD2  | 18       | 0.2           |
| (1,3275) | 1:26:A:TYR:HA   | 1:27:A:LYS:HD2  | 19       | 0.2           |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 1        | 0.2           |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 13       | 0.2           |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 6        | 0.2           |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 16       | 0.2           |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 11       | 0.2           |
| (1,3045) | 1:12:B:ILE:HG21 | 1:16:B:HIS:HE1  | 12       | 0.2           |
| (1,3045) | 1:12:B:ILE:HG22 | 1:16:B:HIS:HE1  | 12       | 0.2           |
| (1,3045) | 1:12:B:ILE:HG23 | 1:16:B:HIS:HE1  | 12       | 0.2           |
| (1,2991) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HA   | 12       | 0.2           |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 4        | 0.2           |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 5        | 0.2           |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 7        | 0.2           |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 11       | 0.2           |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 20       | 0.2           |
| (1,2563) | 1:31:A:LYS:HG3  | 1:32:A:GLU:HG3  | 15       | 0.2           |
| (1,2520) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG3  | 12       | 0.2           |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 17       | 0.2           |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 18       | 0.2           |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 18       | 0.2           |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 18       | 0.2           |
| (1,2110) | 1:63:B:GLU:HB2  | 1:64:B:ASN:HD21 | 11       | 0.2           |
| (1,2103) | 1:63:A:GLU:HB2  | 1:64:A:ASN:HD21 | 17       | 0.2           |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 16       | 0.2           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 8        | 0.2           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 8        | 0.2           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 8        | 0.2           |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 3        | 0.2           |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 3        | 0.2           |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 3        | 0.2           |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 11       | 0.2           |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 11       | 0.2           |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 11       | 0.2           |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 11       | 0.2           |
| (1,1278) | 1:89:B:PHE:HB2  | 1:90:B:TRP:HD1  | 13       | 0.2           |
| (1,1253) | 1:56:B:LYS:H    | 1:56:B:LYS:HD2  | 2        | 0.2           |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 7        | 0.2           |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 7        | 0.2           |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 7        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 18       | 0.2           |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 18       | 0.2           |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 18       | 0.2           |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 19       | 0.2           |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 19       | 0.2           |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 19       | 0.2           |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 15       | 0.2           |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 15       | 0.2           |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 15       | 0.2           |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 17       | 0.2           |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 17       | 0.2           |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 17       | 0.2           |
| (1,1016) | 1:16:B:HIS:HE1  | 1:26:B:TYR:HD1  | 18       | 0.2           |
| (1,1010) | 1:16:A:HIS:HE1  | 1:26:A:TYR:HD1  | 8        | 0.2           |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 20       | 0.2           |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 20       | 0.2           |
| (1,967)  | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 2        | 0.2           |
| (1,967)  | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 2        | 0.2           |
| (1,967)  | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 2        | 0.2           |
| (1,963)  | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 2        | 0.2           |
| (1,938)  | 1:25:A:LYS:HB2  | 1:26:A:TYR:HD1  | 4        | 0.2           |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 7        | 0.2           |
| (1,788)  | 1:49:B:LYS:HB3  | 1:49:B:LYS:HE3  | 19       | 0.2           |
| (1,726)  | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD11 | 2        | 0.2           |
| (1,726)  | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD12 | 2        | 0.2           |
| (1,726)  | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD13 | 2        | 0.2           |
| (1,575)  | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 11       | 0.2           |
| (1,575)  | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 11       | 0.2           |
| (1,575)  | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 11       | 0.2           |
| (1,559)  | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 1        | 0.2           |
| (1,559)  | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 1        | 0.2           |
| (1,559)  | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 1        | 0.2           |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 7        | 0.2           |
| (1,545)  | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 18       | 0.2           |
| (1,538)  | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 1        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 1        | 0.2           |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 1        | 0.2           |
| (1,515) | 1:44:B:PHE:HA   | 1:44:B:PHE:HD2  | 18       | 0.2           |
| (1,499) | 1:57:A:VAL:HG21 | 1:81:A:LEU:HG   | 11       | 0.2           |
| (1,499) | 1:57:A:VAL:HG22 | 1:81:A:LEU:HG   | 11       | 0.2           |
| (1,499) | 1:57:A:VAL:HG23 | 1:81:A:LEU:HG   | 11       | 0.2           |
| (1,454) | 1:30:A:LYS:HD3  | 1:65:A:GLY:HA2  | 20       | 0.2           |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 1        | 0.2           |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 1        | 0.2           |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 1        | 0.2           |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 13       | 0.2           |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 13       | 0.2           |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 13       | 0.2           |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 6        | 0.2           |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 6        | 0.2           |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 6        | 0.2           |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 20       | 0.2           |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 3        | 0.2           |
| (1,395) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 10       | 0.2           |
| (1,395) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 12       | 0.2           |
| (1,390) | 1:30:B:LYS:HG3  | 1:65:B:GLY:HA3  | 11       | 0.2           |
| (1,369) | 1:51:B:VAL:HG11 | 1:53:B:ALA:HB1  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG11 | 1:53:B:ALA:HB2  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG11 | 1:53:B:ALA:HB3  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG12 | 1:53:B:ALA:HB1  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG12 | 1:53:B:ALA:HB2  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG12 | 1:53:B:ALA:HB3  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG13 | 1:53:B:ALA:HB1  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG13 | 1:53:B:ALA:HB2  | 10       | 0.2           |
| (1,369) | 1:51:B:VAL:HG13 | 1:53:B:ALA:HB3  | 10       | 0.2           |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 4        | 0.2           |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 4        | 0.2           |
| (1,311) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HD2  | 18       | 0.2           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 19       | 0.2           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 19       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,276)  | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 19       | 0.2           |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 19       | 0.2           |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 19       | 0.2           |
| (1,276)  | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 19       | 0.2           |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 19       | 0.2           |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 19       | 0.2           |
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 19       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 15       | 0.2           |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 15       | 0.2           |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 2        | 0.2           |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 2        | 0.2           |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 2        | 0.2           |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 10       | 0.2           |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 10       | 0.2           |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 10       | 0.2           |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 2        | 0.2           |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 5        | 0.19          |
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 20       | 0.19          |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 4        | 0.19          |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 16       | 0.19          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 13       | 0.19          |
| (1,3553) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HE2  | 17       | 0.19          |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 2        | 0.19          |
| (1,3516) | 1:89:A:PHE:H    | 1:89:A:PHE:HE2  | 15       | 0.19          |
| (1,3476) | 1:51:A:VAL:H    | 1:55:A:ASP:H    | 3        | 0.19          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 8        | 0.19          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 8        | 0.19          |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 10       | 0.19          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 9        | 0.19          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 17       | 0.19          |
| (1,3279) | 1:26:B:TYR:HA   | 1:27:B:LYS:HD2  | 19       | 0.19          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 19       | 0.19          |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 4        | 0.19          |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 5        | 0.19          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 18       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 10       | 0.19          |
| (1,3128) | 1:86:B:ASN:HB3  | 1:89:B:PHE:HD2  | 4        | 0.19          |
| (1,3125) | 1:86:A:ASN:HB3  | 1:89:A:PHE:HD2  | 20       | 0.19          |
| (1,2941) | 1:30:A:LYS:HD3  | 1:67:A:GLY:H    | 1        | 0.19          |
| (1,2911) | 1:19:A:SER:HB2  | 1:28:A:LEU:HB2  | 6        | 0.19          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 1        | 0.19          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 6        | 0.19          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 14       | 0.19          |
| (1,2571) | 1:31:B:LYS:HG3  | 1:32:B:GLU:HG3  | 8        | 0.19          |
| (1,2370) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG2  | 18       | 0.19          |
| (1,2346) | 1:21:A:LYS:HG3  | 1:32:A:GLU:HB3  | 20       | 0.19          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 18       | 0.19          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 18       | 0.19          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 18       | 0.19          |
| (1,2026) | 1:86:B:ASN:HA   | 1:86:B:ASN:HD21 | 14       | 0.19          |
| (1,1593) | 1:25:B:LYS:HB2  | 1:25:B:LYS:HE3  | 1        | 0.19          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 15       | 0.19          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 18       | 0.19          |
| (1,1588) | 1:25:A:LYS:HB2  | 1:25:A:LYS:HE3  | 5        | 0.19          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 4        | 0.19          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 4        | 0.19          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 4        | 0.19          |
| (1,1565) | 1:22:B:GLU:HB3  | 1:31:B:LYS:HD2  | 10       | 0.19          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 6        | 0.19          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 6        | 0.19          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 6        | 0.19          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 10       | 0.19          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 10       | 0.19          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 10       | 0.19          |
| (1,1395) | 1:31:B:LYS:HB2  | 1:32:B:GLU:H    | 14       | 0.19          |
| (1,1359) | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG3  | 8        | 0.19          |
| (1,1359) | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG3  | 8        | 0.19          |
| (1,1359) | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG3  | 8        | 0.19          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 5        | 0.19          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 5        | 0.19          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 10       | 0.19          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 10       | 0.19          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 10       | 0.19          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 13       | 0.19          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 13       | 0.19          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 13       | 0.19          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 12       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 12       | 0.19          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 12       | 0.19          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 17       | 0.19          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 17       | 0.19          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 17       | 0.19          |
| (1,987)  | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG11 | 14       | 0.19          |
| (1,987)  | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG12 | 14       | 0.19          |
| (1,987)  | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG13 | 14       | 0.19          |
| (1,963)  | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 13       | 0.19          |
| (1,956)  | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 4        | 0.19          |
| (1,956)  | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 4        | 0.19          |
| (1,956)  | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 4        | 0.19          |
| (1,927)  | 1:21:B:LYS:HA   | 1:21:B:LYS:HE2  | 3        | 0.19          |
| (1,918)  | 1:31:A:LYS:H    | 1:31:A:LYS:HG2  | 17       | 0.19          |
| (1,853)  | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG2  | 8        | 0.19          |
| (1,853)  | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG2  | 8        | 0.19          |
| (1,853)  | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG2  | 8        | 0.19          |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 3        | 0.19          |
| (1,688)  | 1:57:B:VAL:HG11 | 1:81:B:LEU:HG   | 16       | 0.19          |
| (1,688)  | 1:57:B:VAL:HG12 | 1:81:B:LEU:HG   | 16       | 0.19          |
| (1,688)  | 1:57:B:VAL:HG13 | 1:81:B:LEU:HG   | 16       | 0.19          |
| (1,566)  | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 3        | 0.19          |
| (1,566)  | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 3        | 0.19          |
| (1,566)  | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 3        | 0.19          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 3        | 0.19          |
| (1,553)  | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 7        | 0.19          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 14       | 0.19          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 14       | 0.19          |
| (1,534)  | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 14       | 0.19          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE2  | 16       | 0.19          |
| (1,524)  | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE3  | 16       | 0.19          |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD11  | 7        | 0.19          |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD12  | 7        | 0.19          |
| (1,441)  | 1:4:A:LEU:HA    | 1:4:A:LEU:HD13  | 7        | 0.19          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 9        | 0.19          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 9        | 0.19          |
| (1,431)  | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 9        | 0.19          |
| (1,429)  | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 1        | 0.19          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 6        | 0.19          |
| (1,407)  | 1:26:B:TYR:HA   | 1:26:B:TYR:HD1  | 9        | 0.19          |
| (1,399)  | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 2        | 0.19          |
| (1,399)  | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 8        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,390) | 1:30:B:LYS:HG3  | 1:65:B:GLY:HA3  | 6        | 0.19          |
| (1,390) | 1:30:B:LYS:HG3  | 1:65:B:GLY:HA3  | 19       | 0.19          |
| (1,389) | 1:29:B:SER:HB2  | 1:31:B:LYS:HD2  | 5        | 0.19          |
| (1,385) | 1:29:A:SER:HB2  | 1:31:A:LYS:HD2  | 7        | 0.19          |
| (1,348) | 1:12:B:ILE:HG21 | 1:16:B:HIS:HD2  | 16       | 0.19          |
| (1,348) | 1:12:B:ILE:HG22 | 1:16:B:HIS:HD2  | 16       | 0.19          |
| (1,348) | 1:12:B:ILE:HG23 | 1:16:B:HIS:HD2  | 16       | 0.19          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 3        | 0.19          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 3        | 0.19          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 2        | 0.19          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 2        | 0.19          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 15       | 0.19          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 15       | 0.19          |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2  | 4        | 0.19          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2  | 4        | 0.19          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2  | 4        | 0.19          |
| (1,259) | 1:37:A:LEU:HD21 | 1:41:A:LEU:HB2  | 10       | 0.19          |
| (1,259) | 1:37:A:LEU:HD22 | 1:41:A:LEU:HB2  | 10       | 0.19          |
| (1,259) | 1:37:A:LEU:HD23 | 1:41:A:LEU:HB2  | 10       | 0.19          |
| (1,201) | 1:42:A:SER:H    | 1:1:B:GLY:HA2   | 2        | 0.19          |
| (1,201) | 1:42:A:SER:H    | 1:1:B:GLY:HA3   | 2        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,176)  | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 3        | 0.19          |
| (1,176)  | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 4        | 0.19          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 9        | 0.19          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 9        | 0.19          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 9        | 0.19          |
| (1,165)  | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 2        | 0.19          |
| (1,165)  | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 2        | 0.19          |
| (1,165)  | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 2        | 0.19          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 12       | 0.19          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 12       | 0.19          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 6        | 0.19          |
| (1,73)   | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG11 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG12 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG13 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG11 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG12 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG13 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG11 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG12 | 17       | 0.19          |
| (1,73)   | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG13 | 17       | 0.19          |
| (1,39)   | 1:4:A:LEU:HD21  | 1:40:B:GLU:HA   | 5        | 0.19          |
| (1,39)   | 1:4:A:LEU:HD22  | 1:40:B:GLU:HA   | 5        | 0.19          |
| (1,39)   | 1:4:A:LEU:HD23  | 1:40:B:GLU:HA   | 5        | 0.19          |
| (1,3614) | 1:58:B:MET:HG2  | 1:60:B:GLU:H    | 12       | 0.18          |
| (1,3604) | 1:51:B:VAL:H    | 1:55:B:ASP:H    | 2        | 0.18          |
| (1,3591) | 1:47:B:ALA:H    | 1:48:B:GLN:HB3  | 6        | 0.18          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 7        | 0.18          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 7        | 0.18          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 7        | 0.18          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 12       | 0.18          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 9        | 0.18          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 14       | 0.18          |
| (1,3278) | 1:90:A:TRP:HE1  | 1:91:A:GLU:H    | 2        | 0.18          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 15       | 0.18          |
| (1,3177) | 1:27:A:LYS:HE3  | 1:71:A:PHE:H    | 3        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3133) | 1:57:A:VAL:H    | 1:58:A:MET:HB3  | 6        | 0.18          |
| (1,2917) | 1:19:B:SER:HB2  | 1:28:B:LEU:HB2  | 20       | 0.18          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 11       | 0.18          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 1        | 0.18          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 8        | 0.18          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 4        | 0.18          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 6        | 0.18          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 13       | 0.18          |
| (1,2563) | 1:31:A:LYS:HG3  | 1:32:A:GLU:HG3  | 19       | 0.18          |
| (1,2517) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG3  | 8        | 0.18          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 9        | 0.18          |
| (1,2401) | 1:1:B:GLY:HA2   | 1:5:B:GLU:HB3   | 9        | 0.18          |
| (1,2364) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG2  | 13       | 0.18          |
| (1,2304) | 1:29:B:SER:HA   | 1:31:B:LYS:HG2  | 13       | 0.18          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 10       | 0.18          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 10       | 0.18          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 10       | 0.18          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 13       | 0.18          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 13       | 0.18          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 13       | 0.18          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD21  | 17       | 0.18          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD22  | 17       | 0.18          |
| (1,1923) | 1:2:A:SER:HA    | 1:4:A:LEU:HD23  | 17       | 0.18          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 6        | 0.18          |
| (1,1637) | 1:27:B:LYS:HE3  | 1:68:B:GLU:HB3  | 11       | 0.18          |
| (1,1592) | 1:25:B:LYS:HE3  | 1:26:B:TYR:HE1  | 10       | 0.18          |
| (1,1504) | 1:76:B:VAL:HG21 | 1:80:B:ALA:H    | 16       | 0.18          |
| (1,1504) | 1:76:B:VAL:HG22 | 1:80:B:ALA:H    | 16       | 0.18          |
| (1,1504) | 1:76:B:VAL:HG23 | 1:80:B:ALA:H    | 16       | 0.18          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 1        | 0.18          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 1        | 0.18          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 1        | 0.18          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 17       | 0.18          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 17       | 0.18          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 17       | 0.18          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 1        | 0.18          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 1        | 0.18          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 1        | 0.18          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 6        | 0.18          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 6        | 0.18          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 6        | 0.18          |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 6        | 0.18          |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 7        | 0.18          |
| (1,1391) | 1:31:A:LYS:HB2  | 1:32:A:GLU:H    | 10       | 0.18          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 17       | 0.18          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 11       | 0.18          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 11       | 0.18          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 11       | 0.18          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 19       | 0.18          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 19       | 0.18          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 19       | 0.18          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 15       | 0.18          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 15       | 0.18          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 15       | 0.18          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 18       | 0.18          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 18       | 0.18          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 18       | 0.18          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 13       | 0.18          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 13       | 0.18          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 13       | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 1        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 6        | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 18       | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 18       | 0.18          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 18       | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 18       | 0.18          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 18       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 18       | 0.18          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 18       | 0.18          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 18       | 0.18          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 18       | 0.18          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 5        | 0.18          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 5        | 0.18          |
| (1,972) | 1:86:B:ASN:HA   | 1:89:B:PHE:HB2  | 6        | 0.18          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 12       | 0.18          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 12       | 0.18          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 12       | 0.18          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 13       | 0.18          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 13       | 0.18          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 13       | 0.18          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 18       | 0.18          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 18       | 0.18          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 18       | 0.18          |
| (1,918) | 1:31:A:LYS:H    | 1:31:A:LYS:HG2  | 5        | 0.18          |
| (1,792) | 1:39:A:THR:H    | 1:39:A:THR:HG21 | 15       | 0.18          |
| (1,792) | 1:39:A:THR:H    | 1:39:A:THR:HG22 | 15       | 0.18          |
| (1,792) | 1:39:A:THR:H    | 1:39:A:THR:HG23 | 15       | 0.18          |
| (1,780) | 1:49:A:LYS:HB3  | 1:49:A:LYS:HE3  | 9        | 0.18          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 16       | 0.18          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 16       | 0.18          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 16       | 0.18          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 12       | 0.18          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 18       | 0.18          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG11 | 1        | 0.18          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG12 | 1        | 0.18          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG13 | 1        | 0.18          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 7        | 0.18          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 7        | 0.18          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 17       | 0.18          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 17       | 0.18          |
| (1,482) | 1:89:B:PHE:HA   | 1:89:B:PHE:HD1  | 18       | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 7        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 7        | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 7        | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 10       | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 10       | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 10       | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 15       | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 15       | 0.18          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 15       | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD11  | 3        | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD12  | 3        | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD13  | 3        | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD11  | 8        | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD12  | 8        | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD13  | 8        | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD11  | 20       | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD12  | 20       | 0.18          |
| (1,441) | 1:4:A:LEU:HA    | 1:4:A:LEU:HD13  | 20       | 0.18          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 14       | 0.18          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 14       | 0.18          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 14       | 0.18          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 16       | 0.18          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 16       | 0.18          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 16       | 0.18          |
| (1,435) | 1:26:B:TYR:HB2  | 1:26:B:TYR:HD2  | 12       | 0.18          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 11       | 0.18          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 11       | 0.18          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 11       | 0.18          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 9        | 0.18          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 10       | 0.18          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 12       | 0.18          |
| (1,390) | 1:30:B:LYS:HG3  | 1:65:B:GLY:HA3  | 12       | 0.18          |
| (1,386) | 1:30:A:LYS:HG3  | 1:65:A:GLY:HA3  | 8        | 0.18          |
| (1,339) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HD2  | 11       | 0.18          |
| (1,339) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HD2  | 11       | 0.18          |
| (1,339) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HD2  | 11       | 0.18          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 6        | 0.18          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 6        | 0.18          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 6        | 0.18          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 6        | 0.18          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 6        | 0.18          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 6        | 0.18          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 6        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 6        | 0.18          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 6        | 0.18          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 17       | 0.18          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 1        | 0.18          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 17       | 0.18          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 17       | 0.18          |
| (1,314) | 1:56:B:LYS:HB2  | 1:56:B:LYS:HD2  | 4        | 0.18          |
| (1,311) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HD2  | 3        | 0.18          |
| (1,277) | 1:61:A:LEU:HA   | 1:61:A:LEU:HD11 | 5        | 0.18          |
| (1,277) | 1:61:A:LEU:HA   | 1:61:A:LEU:HD12 | 5        | 0.18          |
| (1,277) | 1:61:A:LEU:HA   | 1:61:A:LEU:HD13 | 5        | 0.18          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 16       | 0.18          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 16       | 0.18          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 16       | 0.18          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 16       | 0.18          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 16       | 0.18          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 16       | 0.18          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 16       | 0.18          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 16       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,276)  | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 16       | 0.18          |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 9        | 0.18          |
| (1,274)  | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 9        | 0.18          |
| (1,207)  | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1  | 13       | 0.18          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 1        | 0.18          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 1        | 0.18          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 1        | 0.18          |
| (1,166)  | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 6        | 0.18          |
| (1,166)  | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 6        | 0.18          |
| (1,166)  | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 6        | 0.18          |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 19       | 0.18          |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 19       | 0.18          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 15       | 0.18          |
| (1,69)   | 1:72:A:GLN:HG2  | 1:83:B:VAL:HG11 | 9        | 0.18          |
| (1,69)   | 1:72:A:GLN:HG2  | 1:83:B:VAL:HG12 | 9        | 0.18          |
| (1,69)   | 1:72:A:GLN:HG2  | 1:83:B:VAL:HG13 | 9        | 0.18          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 5        | 0.18          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 5        | 0.18          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 5        | 0.18          |
| (1,3620) | 1:68:B:GLU:HB3  | 1:70:B:ASP:HB3  | 16       | 0.17          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 11       | 0.17          |
| (1,3615) | 1:58:B:MET:HG2  | 1:59:B:LYS:HB2  | 17       | 0.17          |
| (1,3605) | 1:51:B:VAL:HB   | 1:52:B:ASP:HB3  | 8        | 0.17          |
| (1,3591) | 1:47:B:ALA:H    | 1:48:B:GLN:HB3  | 10       | 0.17          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 3        | 0.17          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 3        | 0.17          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 3        | 0.17          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 10       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3548) | 1:19:B:SER:HB3 | 1:25:B:LYS:HB2  | 9        | 0.17          |
| (1,3548) | 1:19:B:SER:HB3 | 1:25:B:LYS:HB2  | 11       | 0.17          |
| (1,3528) | 1:9:B:GLU:HA   | 1:71:B:PHE:HE2  | 4        | 0.17          |
| (1,3490) | 1:63:A:GLU:HG3 | 1:64:A:ASN:HB2  | 2        | 0.17          |
| (1,3490) | 1:63:A:GLU:HG3 | 1:64:A:ASN:HB2  | 18       | 0.17          |
| (1,3487) | 1:58:A:MET:HG2 | 1:59:A:LYS:HB2  | 10       | 0.17          |
| (1,3444) | 1:34:A:LYS:HA  | 1:36:A:LEU:HD21 | 4        | 0.17          |
| (1,3444) | 1:34:A:LYS:HA  | 1:36:A:LEU:HD22 | 4        | 0.17          |
| (1,3444) | 1:34:A:LYS:HA  | 1:36:A:LEU:HD23 | 4        | 0.17          |
| (1,3428) | 1:27:A:LYS:HE3 | 1:69:A:VAL:H    | 6        | 0.17          |
| (1,3426) | 1:27:A:LYS:HB3 | 1:70:A:ASP:HB3  | 20       | 0.17          |
| (1,3400) | 1:9:A:GLU:HA   | 1:71:A:PHE:HE2  | 12       | 0.17          |
| (1,3390) | 1:37:B:LEU:HA  | 1:40:B:GLU:HA   | 14       | 0.17          |
| (1,3385) | 1:66:A:ASP:HB2 | 1:68:A:GLU:H    | 19       | 0.17          |
| (1,3383) | 1:37:A:LEU:HA  | 1:40:A:GLU:HA   | 15       | 0.17          |
| (1,3367) | 1:13:A:ASN:H   | 1:16:A:HIS:HD2  | 12       | 0.17          |
| (1,3294) | 1:59:A:LYS:H   | 1:61:A:LEU:HD21 | 5        | 0.17          |
| (1,3294) | 1:59:A:LYS:H   | 1:61:A:LEU:HD22 | 5        | 0.17          |
| (1,3294) | 1:59:A:LYS:H   | 1:61:A:LEU:HD23 | 5        | 0.17          |
| (1,3278) | 1:90:A:TRP:HE1 | 1:91:A:GLU:H    | 20       | 0.17          |
| (1,3128) | 1:86:B:ASN:HB3 | 1:89:B:PHE:HD2  | 20       | 0.17          |
| (1,2601) | 1:22:A:GLU:HB2 | 1:31:A:LYS:HD3  | 17       | 0.17          |
| (1,2472) | 1:59:A:LYS:HG3 | 1:60:A:GLU:HB2  | 10       | 0.17          |
| (1,2472) | 1:59:A:LYS:HG3 | 1:60:A:GLU:HB2  | 19       | 0.17          |
| (1,2454) | 1:30:B:LYS:HG2 | 1:31:B:LYS:HE2  | 13       | 0.17          |
| (1,2364) | 1:90:A:TRP:HA  | 1:91:A:GLU:HG2  | 3        | 0.17          |
| (1,2239) | 1:30:B:LYS:H   | 1:30:B:LYS:HG2  | 10       | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG21 | 2        | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG22 | 2        | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG23 | 2        | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG21 | 8        | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG22 | 8        | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG23 | 8        | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG21 | 19       | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG22 | 19       | 0.17          |
| (1,2151) | 1:37:B:LEU:HA  | 1:39:B:THR:HG23 | 19       | 0.17          |
| (1,2139) | 1:37:A:LEU:HA  | 1:39:A:THR:HG21 | 6        | 0.17          |
| (1,2139) | 1:37:A:LEU:HA  | 1:39:A:THR:HG22 | 6        | 0.17          |
| (1,2139) | 1:37:A:LEU:HA  | 1:39:A:THR:HG23 | 6        | 0.17          |
| (1,2137) | 1:35:A:GLU:H   | 1:35:A:GLU:HG2  | 4        | 0.17          |
| (1,2128) | 1:64:B:ASN:HB3 | 1:73:B:GLU:HB2  | 4        | 0.17          |
| (1,1678) | 1:30:B:LYS:HA  | 1:33:B:LEU:HB3  | 17       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 16       | 0.17          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 16       | 0.17          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 16       | 0.17          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD21  | 5        | 0.17          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD22  | 5        | 0.17          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD23  | 5        | 0.17          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 7        | 0.17          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 7        | 0.17          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 7        | 0.17          |
| (1,1559) | 1:22:A:GLU:HB3  | 1:31:A:LYS:HD2  | 14       | 0.17          |
| (1,1499) | 1:36:B:LEU:HD11 | 1:74:B:TYR:HD1  | 16       | 0.17          |
| (1,1499) | 1:36:B:LEU:HD12 | 1:74:B:TYR:HD1  | 16       | 0.17          |
| (1,1499) | 1:36:B:LEU:HD13 | 1:74:B:TYR:HD1  | 16       | 0.17          |
| (1,1497) | 1:76:A:VAL:HG21 | 1:80:A:ALA:H    | 6        | 0.17          |
| (1,1497) | 1:76:A:VAL:HG22 | 1:80:A:ALA:H    | 6        | 0.17          |
| (1,1497) | 1:76:A:VAL:HG23 | 1:80:A:ALA:H    | 6        | 0.17          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2  | 9        | 0.17          |
| (1,1359) | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG3  | 15       | 0.17          |
| (1,1359) | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG3  | 15       | 0.17          |
| (1,1359) | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG3  | 15       | 0.17          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 16       | 0.17          |
| (1,1275) | 1:21:B:LYS:HB2  | 1:32:B:GLU:HG3  | 8        | 0.17          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 18       | 0.17          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 18       | 0.17          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 18       | 0.17          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 20       | 0.17          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 20       | 0.17          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 20       | 0.17          |
| (1,1221) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HB2  | 18       | 0.17          |
| (1,1052) | 1:27:A:LYS:HE3  | 1:70:A:ASP:HA   | 6        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 2        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 2        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 2        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 3        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 3        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 3        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 4        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 4        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 4        | 0.17          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 14       | 0.17          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 14       | 0.17          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 14       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 10       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 10       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 10       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 11       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 11       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 11       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 20       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 20       | 0.17          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 20       | 0.17          |
| (1,1034) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HA   | 9        | 0.17          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 10       | 0.17          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 10       | 0.17          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 10       | 0.17          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 5        | 0.17          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 5        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 8        | 0.17          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 8        | 0.17          |
| (1,972)  | 1:86:B:ASN:HA   | 1:89:B:PHE:HB2  | 4        | 0.17          |
| (1,972)  | 1:86:B:ASN:HA   | 1:89:B:PHE:HB2  | 13       | 0.17          |
| (1,863)  | 1:11:A:LEU:HA   | 1:14:A:VAL:HB   | 3        | 0.17          |
| (1,852)  | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 6        | 0.17          |
| (1,839)  | 1:38:B:GLN:HA   | 1:45:B:LEU:HD21 | 17       | 0.17          |
| (1,839)  | 1:38:B:GLN:HA   | 1:45:B:LEU:HD22 | 17       | 0.17          |
| (1,839)  | 1:38:B:GLN:HA   | 1:45:B:LEU:HD23 | 17       | 0.17          |
| (1,832)  | 1:38:A:GLN:HA   | 1:45:A:LEU:HD21 | 10       | 0.17          |
| (1,832)  | 1:38:A:GLN:HA   | 1:45:A:LEU:HD22 | 10       | 0.17          |
| (1,832)  | 1:38:A:GLN:HA   | 1:45:A:LEU:HD23 | 10       | 0.17          |
| (1,678)  | 1:57:A:VAL:HG11 | 1:81:A:LEU:HG   | 16       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,678) | 1:57:A:VAL:HG12 | 1:81:A:LEU:HG   | 16       | 0.17          |
| (1,678) | 1:57:A:VAL:HG13 | 1:81:A:LEU:HG   | 16       | 0.17          |
| (1,575) | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 20       | 0.17          |
| (1,575) | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 20       | 0.17          |
| (1,575) | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 20       | 0.17          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 6        | 0.17          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 16       | 0.17          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 5        | 0.17          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 5        | 0.17          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 5        | 0.17          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 15       | 0.17          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 15       | 0.17          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 15       | 0.17          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 4        | 0.17          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 10       | 0.17          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 14       | 0.17          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 17       | 0.17          |
| (1,395) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 9        | 0.17          |
| (1,387) | 1:60:A:GLU:HA   | 1:60:A:GLU:HG3  | 2        | 0.17          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 12       | 0.17          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 12       | 0.17          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 4        | 0.17          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 4        | 0.17          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 10       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 10       | 0.17          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 13       | 0.17          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 13       | 0.17          |
| (1,314) | 1:56:B:LYS:HB2  | 1:56:B:LYS:HD2  | 18       | 0.17          |
| (1,311) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HD2  | 7        | 0.17          |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB1  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB2  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB3  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB1  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB2  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB3  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB1  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB2  | 6        | 0.17          |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB3  | 6        | 0.17          |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB1  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB2  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB3  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB1  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB2  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB3  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB1  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB2  | 16       | 0.17          |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB3  | 16       | 0.17          |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2  | 3        | 0.17          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2  | 3        | 0.17          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2  | 3        | 0.17          |
| (1,201) | 1:42:A:SER:H    | 1:1:B:GLY:HA2   | 1        | 0.17          |
| (1,201) | 1:42:A:SER:H    | 1:1:B:GLY:HA3   | 1        | 0.17          |
| (1,201) | 1:42:A:SER:H    | 1:1:B:GLY:HA2   | 20       | 0.17          |
| (1,201) | 1:42:A:SER:H    | 1:1:B:GLY:HA3   | 20       | 0.17          |
| (1,166) | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 4        | 0.17          |
| (1,166) | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 4        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,166) | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 4        | 0.17          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 10       | 0.17          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 10       | 0.17          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 10       | 0.17          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 19       | 0.17          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 19       | 0.17          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 19       | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 1        | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 8        | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 10       | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 14       | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 14       | 0.17          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 14       | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 14       | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 14       | 0.17          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 14       | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 14       | 0.17          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 14       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 14       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 9        | 0.17          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 13       | 0.17          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 13       | 0.17          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 11       | 0.17          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 13       | 0.17          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 14       | 0.17          |
| (1,82)   | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB1  | 1        | 0.17          |
| (1,82)   | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB2  | 1        | 0.17          |
| (1,82)   | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB3  | 1        | 0.17          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 18       | 0.17          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 18       | 0.17          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 18       | 0.17          |
| (1,3648) | 1:92:B:ASN:HB3  | 1:93:B:SER:HB2  | 15       | 0.16          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 8        | 0.16          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 8        | 0.16          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 8        | 0.16          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 14       | 0.16          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 14       | 0.16          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 14       | 0.16          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 17       | 0.16          |
| (1,3550) | 1:22:B:GLU:HB2  | 1:29:B:SER:HA   | 5        | 0.16          |
| (1,3550) | 1:22:B:GLU:HB2  | 1:29:B:SER:HA   | 13       | 0.16          |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 1        | 0.16          |
| (1,3533) | 1:14:B:VAL:HA   | 1:74:B:TYR:HE2  | 5        | 0.16          |
| (1,3533) | 1:14:B:VAL:HA   | 1:74:B:TYR:HE2  | 12       | 0.16          |
| (1,3486) | 1:58:A:MET:HG2  | 1:60:A:GLU:H    | 17       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3447) | 1:37:A:LEU:HB2  | 1:74:A:TYR:HA   | 7        | 0.16          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 1        | 0.16          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 1        | 0.16          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 1        | 0.16          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 18       | 0.16          |
| (1,3382) | 1:37:A:LEU:HA   | 1:40:A:GLU:HG3  | 20       | 0.16          |
| (1,3338) | 1:1:B:GLY:HA3   | 1:5:B:GLU:HB3   | 17       | 0.16          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 20       | 0.16          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 10       | 0.16          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 2        | 0.16          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 7        | 0.16          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 12       | 0.16          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 18       | 0.16          |
| (1,3201) | 1:45:A:LEU:HD11 | 1:46:A:ASP:HB3  | 2        | 0.16          |
| (1,3201) | 1:45:A:LEU:HD12 | 1:46:A:ASP:HB3  | 2        | 0.16          |
| (1,3201) | 1:45:A:LEU:HD13 | 1:46:A:ASP:HB3  | 2        | 0.16          |
| (1,2949) | 1:15:B:PHE:HE2  | 1:19:B:SER:HA   | 17       | 0.16          |
| (1,2918) | 1:41:B:LEU:HA   | 1:45:B:LEU:HD21 | 17       | 0.16          |
| (1,2918) | 1:41:B:LEU:HA   | 1:45:B:LEU:HD22 | 17       | 0.16          |
| (1,2918) | 1:41:B:LEU:HA   | 1:45:B:LEU:HD23 | 17       | 0.16          |
| (1,2881) | 1:46:A:ASP:HB2  | 1:49:A:LYS:HG3  | 9        | 0.16          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 9        | 0.16          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 16       | 0.16          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 18       | 0.16          |
| (1,2612) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HD3  | 1        | 0.16          |
| (1,2571) | 1:31:B:LYS:HG3  | 1:32:B:GLU:HG3  | 14       | 0.16          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 4        | 0.16          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 20       | 0.16          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 13       | 0.16          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 16       | 0.16          |
| (1,2370) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG2  | 13       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 3        | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 3        | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 3        | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 7        | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 7        | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 7        | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 10       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 10       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 10       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 11       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 11       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 11       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 14       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 14       | 0.16          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 14       | 0.16          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD21  | 18       | 0.16          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD22  | 18       | 0.16          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD23  | 18       | 0.16          |
| (1,1616) | 1:30:A:LYS:HE2  | 1:33:A:LEU:HB3  | 16       | 0.16          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 13       | 0.16          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 20       | 0.16          |
| (1,1588) | 1:25:A:LYS:HB2  | 1:25:A:LYS:HE3  | 16       | 0.16          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 12       | 0.16          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 12       | 0.16          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 12       | 0.16          |
| (1,1533) | 1:24:B:ASP:HB2  | 1:27:B:LYS:HG2  | 20       | 0.16          |
| (1,1504) | 1:76:B:VAL:HG21 | 1:80:B:ALA:H    | 20       | 0.16          |
| (1,1504) | 1:76:B:VAL:HG22 | 1:80:B:ALA:H    | 20       | 0.16          |
| (1,1504) | 1:76:B:VAL:HG23 | 1:80:B:ALA:H    | 20       | 0.16          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 5        | 0.16          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 5        | 0.16          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 5        | 0.16          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 10       | 0.16          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 10       | 0.16          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 10       | 0.16          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 15       | 0.16          |
| (1,1249) | 1:56:A:LYS:H    | 1:56:A:LYS:HD2  | 11       | 0.16          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 2        | 0.16          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 2        | 0.16          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 2        | 0.16          |
| (1,1230) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HB2  | 7        | 0.16          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 6        | 0.16          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 6        | 0.16          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 6        | 0.16          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 15       | 0.16          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 15       | 0.16          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 15       | 0.16          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 2        | 0.16          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 2        | 0.16          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 2        | 0.16          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 11       | 0.16          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 11       | 0.16          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 11       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 11       | 0.16          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 11       | 0.16          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 11       | 0.16          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 11       | 0.16          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 11       | 0.16          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 11       | 0.16          |
| (1,994) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG11 | 14       | 0.16          |
| (1,994) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG12 | 14       | 0.16          |
| (1,994) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG13 | 14       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 12       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 16       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 20       | 0.16          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 20       | 0.16          |
| (1,972) | 1:86:B:ASN:HA   | 1:89:B:PHE:HB2  | 20       | 0.16          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 8        | 0.16          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 8        | 0.16          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 8        | 0.16          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 15       | 0.16          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 15       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 15       | 0.16          |
| (1,839) | 1:38:B:GLN:HA   | 1:45:B:LEU:HD21 | 14       | 0.16          |
| (1,839) | 1:38:B:GLN:HA   | 1:45:B:LEU:HD22 | 14       | 0.16          |
| (1,839) | 1:38:B:GLN:HA   | 1:45:B:LEU:HD23 | 14       | 0.16          |
| (1,788) | 1:49:B:LYS:HB3  | 1:49:B:LYS:HE3  | 10       | 0.16          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD11 | 20       | 0.16          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD12 | 20       | 0.16          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD13 | 20       | 0.16          |
| (1,684) | 1:38:B:GLN:H    | 1:38:B:GLN:HG2  | 18       | 0.16          |
| (1,603) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HE3  | 2        | 0.16          |
| (1,575) | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 5        | 0.16          |
| (1,575) | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 5        | 0.16          |
| (1,575) | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 5        | 0.16          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 5        | 0.16          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 5        | 0.16          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 5        | 0.16          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 8        | 0.16          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 8        | 0.16          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 8        | 0.16          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 5        | 0.16          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 5        | 0.16          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 5        | 0.16          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 1        | 0.16          |
| (1,549) | 1:3:B:GLU:HA    | 1:3:B:GLU:HG2   | 17       | 0.16          |
| (1,545) | 1:44:A:PHE:HB2  | 1:44:A:PHE:HD1  | 13       | 0.16          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 18       | 0.16          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 18       | 0.16          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 18       | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 2        | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 2        | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 2        | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 10       | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 10       | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 10       | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 18       | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 18       | 0.16          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 18       | 0.16          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 9        | 0.16          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 9        | 0.16          |
| (1,499) | 1:57:A:VAL:HG21 | 1:81:A:LEU:HG   | 15       | 0.16          |
| (1,499) | 1:57:A:VAL:HG22 | 1:81:A:LEU:HG   | 15       | 0.16          |
| (1,499) | 1:57:A:VAL:HG23 | 1:81:A:LEU:HG   | 15       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,479) | 1:89:A:PHE:HA   | 1:89:A:PHE:HD1  | 17       | 0.16          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 4        | 0.16          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 4        | 0.16          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 4        | 0.16          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 19       | 0.16          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 19       | 0.16          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 19       | 0.16          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 3        | 0.16          |
| (1,395) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 18       | 0.16          |
| (1,391) | 1:60:B:GLU:HA   | 1:60:B:GLU:HG3  | 6        | 0.16          |
| (1,390) | 1:30:B:LYS:HG3  | 1:65:B:GLY:HA3  | 13       | 0.16          |
| (1,387) | 1:60:A:GLU:HA   | 1:60:A:GLU:HG3  | 3        | 0.16          |
| (1,387) | 1:60:A:GLU:HA   | 1:60:A:GLU:HG3  | 12       | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 5        | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 16       | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 17       | 0.16          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 17       | 0.16          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 2        | 0.16          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 2        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 2        | 0.16          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 2        | 0.16          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 2        | 0.16          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 2        | 0.16          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 2        | 0.16          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 2        | 0.16          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 2        | 0.16          |
| (1,314) | 1:56:B:LYS:HB2  | 1:56:B:LYS:HD2  | 7        | 0.16          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 3        | 0.16          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 3        | 0.16          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 3        | 0.16          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 4        | 0.16          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 4        | 0.16          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 4        | 0.16          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 8        | 0.16          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 18       | 0.16          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 18       | 0.16          |
| (1,250) | 1:86:A:ASN:HD22 | 1:9:B:GLU:HB2   | 4        | 0.16          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 19       | 0.16          |
| (1,168) | 1:83:A:VAL:HG11 | 1:72:B:GLN:HG3  | 20       | 0.16          |
| (1,168) | 1:83:A:VAL:HG12 | 1:72:B:GLN:HG3  | 20       | 0.16          |
| (1,168) | 1:83:A:VAL:HG13 | 1:72:B:GLN:HG3  | 20       | 0.16          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 7        | 0.16          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 7        | 0.16          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 7        | 0.16          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 2        | 0.16          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 2        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 2        | 0.16          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 2        | 0.16          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 2        | 0.16          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 2        | 0.16          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 2        | 0.16          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 2        | 0.16          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 2        | 0.16          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 10       | 0.16          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 10       | 0.16          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 9        | 0.16          |
| (1,81)   | 1:72:A:GLN:HA   | 1:80:B:ALA:HA   | 3        | 0.16          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 6        | 0.16          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 6        | 0.16          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 6        | 0.16          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 16       | 0.16          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 16       | 0.16          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 16       | 0.16          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 6        | 0.16          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 6        | 0.16          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 6        | 0.16          |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 9        | 0.16          |
| (1,3648) | 1:92:B:ASN:HB3  | 1:93:B:SER:HB2  | 20       | 0.15          |
| (1,3642) | 1:86:B:ASN:HB2  | 1:87:B:ASN:HB2  | 19       | 0.15          |
| (1,3617) | 1:63:B:GLU:HA   | 1:66:B:ASP:HB2  | 17       | 0.15          |
| (1,3598) | 1:48:B:GLN:HE22 | 1:49:B:LYS:H    | 3        | 0.15          |
| (1,3575) | 1:37:B:LEU:HB2  | 1:74:B:TYR:HA   | 10       | 0.15          |
| (1,3575) | 1:37:B:LEU:HB2  | 1:74:B:TYR:HA   | 15       | 0.15          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 12       | 0.15          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 12       | 0.15          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 12       | 0.15          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 17       | 0.15          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 17       | 0.15          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 17       | 0.15          |
| (1,3549) | 1:20:B:GLY:HA3  | 1:21:B:LYS:HE2  | 6        | 0.15          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 6        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3491) | 1:64:A:ASN:HB3  | 1:67:A:GLY:H    | 14       | 0.15          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 4        | 0.15          |
| (1,3489) | 1:63:A:GLU:HA   | 1:66:A:ASP:HB2  | 20       | 0.15          |
| (1,3447) | 1:37:A:LEU:HB2  | 1:74:A:TYR:HA   | 9        | 0.15          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 8        | 0.15          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 8        | 0.15          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 8        | 0.15          |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 4        | 0.15          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 8        | 0.15          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 16       | 0.15          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 17       | 0.15          |
| (1,3400) | 1:9:A:GLU:HA    | 1:71:A:PHE:HE2  | 1        | 0.15          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 5        | 0.15          |
| (1,3279) | 1:26:B:TYR:HA   | 1:27:B:LYS:HD2  | 14       | 0.15          |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 19       | 0.15          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 2        | 0.15          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 14       | 0.15          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 2        | 0.15          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 7        | 0.15          |
| (1,3181) | 1:27:B:LYS:HE3  | 1:71:B:PHE:H    | 14       | 0.15          |
| (1,3118) | 1:34:A:LYS:HG3  | 1:35:A:GLU:H    | 9        | 0.15          |
| (1,3045) | 1:12:B:ILE:HG21 | 1:16:B:HIS:HE1  | 11       | 0.15          |
| (1,3045) | 1:12:B:ILE:HG22 | 1:16:B:HIS:HE1  | 11       | 0.15          |
| (1,3045) | 1:12:B:ILE:HG23 | 1:16:B:HIS:HE1  | 11       | 0.15          |
| (1,2987) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HA   | 11       | 0.15          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 10       | 0.15          |
| (1,2563) | 1:31:A:LYS:HG3  | 1:32:A:GLU:HG3  | 10       | 0.15          |
| (1,2563) | 1:31:A:LYS:HG3  | 1:32:A:GLU:HG3  | 18       | 0.15          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 17       | 0.15          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 8        | 0.15          |
| (1,2234) | 1:30:A:LYS:H    | 1:30:A:LYS:HG2  | 8        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 4        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 4        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 4        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 5        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 5        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 5        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 6        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 6        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 6        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 9        | 0.15          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 9        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 9        | 0.15          |
| (1,2149) | 1:35:B:GLU:H    | 1:35:B:GLU:HG2  | 8        | 0.15          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 4        | 0.15          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 4        | 0.15          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 4        | 0.15          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 16       | 0.15          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 16       | 0.15          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 16       | 0.15          |
| (1,2026) | 1:86:B:ASN:HA   | 1:86:B:ASN:HD21 | 16       | 0.15          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG11 | 20       | 0.15          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG12 | 20       | 0.15          |
| (1,1952) | 1:15:B:PHE:HE1  | 1:69:B:VAL:HG13 | 20       | 0.15          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 15       | 0.15          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 18       | 0.15          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 17       | 0.15          |
| (1,1669) | 1:30:A:LYS:HA   | 1:33:A:LEU:HB3  | 14       | 0.15          |
| (1,1664) | 1:54:B:VAL:HA   | 1:81:B:LEU:HG   | 16       | 0.15          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG11 | 16       | 0.15          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG12 | 16       | 0.15          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG13 | 16       | 0.15          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG11 | 17       | 0.15          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG12 | 17       | 0.15          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG13 | 17       | 0.15          |
| (1,1593) | 1:25:B:LYS:HB2  | 1:25:B:LYS:HE3  | 11       | 0.15          |
| (1,1592) | 1:25:B:LYS:HE3  | 1:26:B:TYR:HE1  | 11       | 0.15          |
| (1,1497) | 1:76:A:VAL:HG21 | 1:80:A:ALA:H    | 20       | 0.15          |
| (1,1497) | 1:76:A:VAL:HG22 | 1:80:A:ALA:H    | 20       | 0.15          |
| (1,1497) | 1:76:A:VAL:HG23 | 1:80:A:ALA:H    | 20       | 0.15          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2  | 6        | 0.15          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 6        | 0.15          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 7        | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 13       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 13       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 13       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 15       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 15       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 15       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 17       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 17       | 0.15          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 17       | 0.15          |
| (1,1230) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HB2  | 1        | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 8        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 8        | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 8        | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 13       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 13       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 13       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 16       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 16       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 16       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 19       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 19       | 0.15          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 19       | 0.15          |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG21 | 19       | 0.15          |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG22 | 19       | 0.15          |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG23 | 19       | 0.15          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 5        | 0.15          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 5        | 0.15          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 5        | 0.15          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 20       | 0.15          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 20       | 0.15          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 20       | 0.15          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 1        | 0.15          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 1        | 0.15          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 1        | 0.15          |
| (1,1031) | 1:45:B:LEU:HD11 | 1:46:B:ASP:HB2  | 20       | 0.15          |
| (1,1031) | 1:45:B:LEU:HD12 | 1:46:B:ASP:HB2  | 20       | 0.15          |
| (1,1031) | 1:45:B:LEU:HD13 | 1:46:B:ASP:HB2  | 20       | 0.15          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 9        | 0.15          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 9        | 0.15          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 3        | 0.15          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 3        | 0.15          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 3        | 0.15          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 3        | 0.15          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 3        | 0.15          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 3        | 0.15          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 3        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 3        | 0.15          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 3        | 0.15          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 4        | 0.15          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 15       | 0.15          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 15       | 0.15          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 19       | 0.15          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 19       | 0.15          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 19       | 0.15          |
| (1,961) | 1:86:A:ASN:HA   | 1:89:A:PHE:HB2  | 7        | 0.15          |
| (1,952) | 1:29:A:SER:HB3  | 1:68:A:GLU:HG3  | 2        | 0.15          |
| (1,952) | 1:29:A:SER:HB3  | 1:68:A:GLU:HG3  | 6        | 0.15          |
| (1,918) | 1:31:A:LYS:H    | 1:31:A:LYS:HG2  | 6        | 0.15          |
| (1,918) | 1:31:A:LYS:H    | 1:31:A:LYS:HG2  | 16       | 0.15          |
| (1,892) | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 1        | 0.15          |
| (1,858) | 1:31:A:LYS:HB3  | 1:31:A:LYS:HE2  | 14       | 0.15          |
| (1,853) | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG2  | 7        | 0.15          |
| (1,853) | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG2  | 7        | 0.15          |
| (1,853) | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG2  | 7        | 0.15          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD21 | 2        | 0.15          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD22 | 2        | 0.15          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD23 | 2        | 0.15          |
| (1,788) | 1:49:B:LYS:HB3  | 1:49:B:LYS:HE3  | 12       | 0.15          |
| (1,688) | 1:57:B:VAL:HG11 | 1:81:B:LEU:HG   | 18       | 0.15          |
| (1,688) | 1:57:B:VAL:HG12 | 1:81:B:LEU:HG   | 18       | 0.15          |
| (1,688) | 1:57:B:VAL:HG13 | 1:81:B:LEU:HG   | 18       | 0.15          |
| (1,674) | 1:38:A:GLN:H    | 1:38:A:GLN:HG2  | 14       | 0.15          |
| (1,659) | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG21 | 20       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,659) | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG22 | 20       | 0.15          |
| (1,659) | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG23 | 20       | 0.15          |
| (1,575) | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 4        | 0.15          |
| (1,575) | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 4        | 0.15          |
| (1,575) | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 4        | 0.15          |
| (1,572) | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 4        | 0.15          |
| (1,572) | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 4        | 0.15          |
| (1,572) | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 4        | 0.15          |
| (1,572) | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 15       | 0.15          |
| (1,572) | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 15       | 0.15          |
| (1,572) | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 15       | 0.15          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 6        | 0.15          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 6        | 0.15          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 6        | 0.15          |
| (1,553) | 1:44:B:PHE:HB2  | 1:44:B:PHE:HD1  | 2        | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 8        | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 8        | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 8        | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 10       | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 10       | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 10       | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 20       | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 20       | 0.15          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 20       | 0.15          |
| (1,524) | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE2  | 2        | 0.15          |
| (1,524) | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE3  | 2        | 0.15          |
| (1,524) | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE2  | 6        | 0.15          |
| (1,524) | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE3  | 6        | 0.15          |
| (1,524) | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE2  | 20       | 0.15          |
| (1,524) | 1:59:B:LYS:HB2  | 1:59:B:LYS:HE3  | 20       | 0.15          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 13       | 0.15          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 13       | 0.15          |
| (1,479) | 1:89:A:PHE:HA   | 1:89:A:PHE:HD1  | 13       | 0.15          |
| (1,460) | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD21 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD22 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD23 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD21 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD22 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD23 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD21 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD22 | 18       | 0.15          |
| (1,460) | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD23 | 18       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 11       | 0.15          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 11       | 0.15          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 11       | 0.15          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 12       | 0.15          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 12       | 0.15          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 12       | 0.15          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 4        | 0.15          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 4        | 0.15          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 4        | 0.15          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG21 | 12       | 0.15          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG22 | 12       | 0.15          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG23 | 12       | 0.15          |
| (1,391) | 1:60:B:GLU:HA   | 1:60:B:GLU:HG3  | 8        | 0.15          |
| (1,389) | 1:29:B:SER:HB2  | 1:31:B:LYS:HD2  | 17       | 0.15          |
| (1,387) | 1:60:A:GLU:HA   | 1:60:A:GLU:HG3  | 16       | 0.15          |
| (1,364) | 1:73:B:GLU:HA   | 1:73:B:GLU:HG3  | 13       | 0.15          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 19       | 0.15          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 19       | 0.15          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 8        | 0.15          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 8        | 0.15          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 9        | 0.15          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 9        | 0.15          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 9        | 0.15          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 9        | 0.15          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 9        | 0.15          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 9        | 0.15          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 9        | 0.15          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 9        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 5        | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 9        | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 14       | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 19       | 0.15          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 19       | 0.15          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 13       | 0.15          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 13       | 0.15          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 13       | 0.15          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 13       | 0.15          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 13       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 13       | 0.15          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 13       | 0.15          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 13       | 0.15          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 13       | 0.15          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 16       | 0.15          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 16       | 0.15          |
| (1,254) | 1:89:A:PHE:HD2  | 1:9:B:GLU:HG2   | 12       | 0.15          |
| (1,250) | 1:86:A:ASN:HD22 | 1:9:B:GLU:HB2   | 3        | 0.15          |
| (1,151) | 1:80:A:ALA:HA   | 1:72:B:GLN:HA   | 14       | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 3        | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 11       | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 17       | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 17       | 0.15          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 17       | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 17       | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 17       | 0.15          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 17       | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 17       | 0.15          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 17       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 17       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 18       | 0.15          |
| (1,137)  | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 18       | 0.15          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 7        | 0.15          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 7        | 0.15          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 8        | 0.15          |
| (1,85)   | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 12       | 0.15          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 8        | 0.15          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 8        | 0.15          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 8        | 0.15          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 18       | 0.15          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 18       | 0.15          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 18       | 0.15          |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 1        | 0.15          |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 20       | 0.15          |
| (1,3642) | 1:86:B:ASN:HB2  | 1:87:B:ASN:HB2  | 2        | 0.14          |
| (1,3620) | 1:68:B:GLU:HB3  | 1:70:B:ASP:HB3  | 12       | 0.14          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 1        | 0.14          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 15       | 0.14          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 19       | 0.14          |
| (1,3617) | 1:63:B:GLU:HA   | 1:66:B:ASP:HB2  | 3        | 0.14          |
| (1,3579) | 1:37:B:LEU:HD21 | 1:40:B:GLU:HA   | 17       | 0.14          |
| (1,3579) | 1:37:B:LEU:HD22 | 1:40:B:GLU:HA   | 17       | 0.14          |
| (1,3579) | 1:37:B:LEU:HD23 | 1:40:B:GLU:HA   | 17       | 0.14          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 7        | 0.14          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 7        | 0.14          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 7        | 0.14          |
| (1,3575) | 1:37:B:LEU:HB2  | 1:74:B:TYR:HA   | 1        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3575) | 1:37:B:LEU:HB2  | 1:74:B:TYR:HA   | 2        | 0.14          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 11       | 0.14          |
| (1,3556) | 1:27:B:LYS:HE3  | 1:69:B:VAL:H    | 9        | 0.14          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 20       | 0.14          |
| (1,3533) | 1:14:B:VAL:HA   | 1:74:B:TYR:HE2  | 16       | 0.14          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 10       | 0.14          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 20       | 0.14          |
| (1,3470) | 1:48:A:GLN:HE22 | 1:49:A:LYS:H    | 1        | 0.14          |
| (1,3452) | 1:37:A:LEU:HD21 | 1:38:A:GLN:HB2  | 2        | 0.14          |
| (1,3452) | 1:37:A:LEU:HD22 | 1:38:A:GLN:HB2  | 2        | 0.14          |
| (1,3452) | 1:37:A:LEU:HD23 | 1:38:A:GLN:HB2  | 2        | 0.14          |
| (1,3447) | 1:37:A:LEU:HB2  | 1:74:A:TYR:HA   | 13       | 0.14          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 2        | 0.14          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 2        | 0.14          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 2        | 0.14          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 7        | 0.14          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 7        | 0.14          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 7        | 0.14          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 15       | 0.14          |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 15       | 0.14          |
| (1,3424) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HE1  | 11       | 0.14          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 6        | 0.14          |
| (1,3390) | 1:37:B:LEU:HA   | 1:40:B:GLU:HA   | 7        | 0.14          |
| (1,3338) | 1:1:B:GLY:HA3   | 1:5:B:GLU:HB3   | 10       | 0.14          |
| (1,3334) | 1:49:A:LYS:H    | 1:50:A:ASP:HB3  | 14       | 0.14          |
| (1,3275) | 1:26:A:TYR:HA   | 1:27:A:LYS:HD2  | 3        | 0.14          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 3        | 0.14          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 4        | 0.14          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 5        | 0.14          |
| (1,3239) | 1:59:B:LYS:H    | 1:60:B:GLU:HB3  | 8        | 0.14          |
| (1,3050) | 1:49:B:LYS:H    | 1:50:B:ASP:HB2  | 1        | 0.14          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 5        | 0.14          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 20       | 0.14          |
| (1,2830) | 1:44:B:PHE:H    | 1:45:B:LEU:HG   | 5        | 0.14          |
| (1,2538) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HA   | 6        | 0.14          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 8        | 0.14          |
| (1,2472) | 1:59:A:LYS:HG3  | 1:60:A:GLU:HB2  | 5        | 0.14          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 5        | 0.14          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 6        | 0.14          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 10       | 0.14          |
| (1,2401) | 1:1:B:GLY:HA2   | 1:5:B:GLU:HB3   | 19       | 0.14          |
| (1,2370) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG2  | 3        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 11       | 0.14          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 11       | 0.14          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 11       | 0.14          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 12       | 0.14          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 12       | 0.14          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 12       | 0.14          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 5        | 0.14          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 5        | 0.14          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 5        | 0.14          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG21 | 19       | 0.14          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG22 | 19       | 0.14          |
| (1,2139) | 1:37:A:LEU:HA   | 1:39:A:THR:HG23 | 19       | 0.14          |
| (1,2082) | 1:25:B:LYS:HG3  | 1:26:B:TYR:H    | 20       | 0.14          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD21 | 11       | 0.14          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD22 | 11       | 0.14          |
| (1,2080) | 1:15:B:PHE:HD1  | 1:36:B:LEU:HD23 | 11       | 0.14          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD21  | 13       | 0.14          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD22  | 13       | 0.14          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD23  | 13       | 0.14          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD21  | 19       | 0.14          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD22  | 19       | 0.14          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD23  | 19       | 0.14          |
| (1,1651) | 1:2:A:SER:HB3   | 1:3:A:GLU:HB2   | 18       | 0.14          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 4        | 0.14          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 4        | 0.14          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 4        | 0.14          |
| (1,1616) | 1:30:A:LYS:HE2  | 1:33:A:LEU:HB3  | 18       | 0.14          |
| (1,1593) | 1:25:B:LYS:HB2  | 1:25:B:LYS:HE3  | 16       | 0.14          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 13       | 0.14          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 13       | 0.14          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 13       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD21 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD22 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD23 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD21 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD22 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD23 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD21 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD22 | 11       | 0.14          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD23 | 11       | 0.14          |
| (1,1359) | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG3  | 12       | 0.14          |
| (1,1359) | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG3  | 12       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1359) | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG3  | 12       | 0.14          |
| (1,1354) | 1:36:A:LEU:HD11 | 1:40:A:GLU:HG3  | 9        | 0.14          |
| (1,1354) | 1:36:A:LEU:HD12 | 1:40:A:GLU:HG3  | 9        | 0.14          |
| (1,1354) | 1:36:A:LEU:HD13 | 1:40:A:GLU:HG3  | 9        | 0.14          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 9        | 0.14          |
| (1,1278) | 1:89:B:PHE:HB2  | 1:90:B:TRP:HD1  | 6        | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 1        | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 1        | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 1        | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 5        | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 5        | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 5        | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 10       | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 10       | 0.14          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 10       | 0.14          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 17       | 0.14          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 17       | 0.14          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 17       | 0.14          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 18       | 0.14          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 18       | 0.14          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 18       | 0.14          |
| (1,1129) | 1:33:B:LEU:HA   | 1:69:B:VAL:HG11 | 12       | 0.14          |
| (1,1129) | 1:33:B:LEU:HA   | 1:69:B:VAL:HG12 | 12       | 0.14          |
| (1,1129) | 1:33:B:LEU:HA   | 1:69:B:VAL:HG13 | 12       | 0.14          |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG21 | 20       | 0.14          |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG22 | 20       | 0.14          |
| (1,1068) | 1:78:B:VAL:H    | 1:78:B:VAL:HG23 | 20       | 0.14          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 8        | 0.14          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 8        | 0.14          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 8        | 0.14          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 12       | 0.14          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 12       | 0.14          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 12       | 0.14          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 3        | 0.14          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 3        | 0.14          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 3        | 0.14          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 7        | 0.14          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 7        | 0.14          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 7        | 0.14          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 7        | 0.14          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 7        | 0.14          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 7        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 7        | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 7        | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 7        | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 12       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 15       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 16       | 0.14          |
| (1,995) | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 16       | 0.14          |
| (1,994) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG11 | 10       | 0.14          |
| (1,994) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG12 | 10       | 0.14          |
| (1,994) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HG13 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 9        | 0.14          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 9        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 10       | 0.14          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 10       | 0.14          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 7        | 0.14          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 7        | 0.14          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 7        | 0.14          |
| (1,963) | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 16       | 0.14          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 14       | 0.14          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 14       | 0.14          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 14       | 0.14          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 20       | 0.14          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 20       | 0.14          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 20       | 0.14          |
| (1,952) | 1:29:A:SER:HB3  | 1:68:A:GLU:HG3  | 1        | 0.14          |
| (1,782) | 1:52:A:ASP:HA   | 1:54:A:VAL:HG11 | 17       | 0.14          |
| (1,782) | 1:52:A:ASP:HA   | 1:54:A:VAL:HG12 | 17       | 0.14          |
| (1,782) | 1:52:A:ASP:HA   | 1:54:A:VAL:HG13 | 17       | 0.14          |
| (1,780) | 1:49:A:LYS:HB3  | 1:49:A:LYS:HE3  | 15       | 0.14          |
| (1,745) | 1:6:A:THR:HG21  | 1:9:A:GLU:HB2   | 6        | 0.14          |
| (1,745) | 1:6:A:THR:HG22  | 1:9:A:GLU:HB2   | 6        | 0.14          |
| (1,745) | 1:6:A:THR:HG23  | 1:9:A:GLU:HB2   | 6        | 0.14          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD11 | 17       | 0.14          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD12 | 17       | 0.14          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD13 | 17       | 0.14          |
| (1,667) | 1:24:B:ASP:HB3  | 1:27:B:LYS:HB2  | 15       | 0.14          |
| (1,575) | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 16       | 0.14          |
| (1,575) | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 16       | 0.14          |
| (1,575) | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 16       | 0.14          |
| (1,572) | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 2        | 0.14          |
| (1,572) | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 2        | 0.14          |
| (1,572) | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 2        | 0.14          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 10       | 0.14          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 10       | 0.14          |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 10       | 0.14          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG11 | 20       | 0.14          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG12 | 20       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG13 | 20       | 0.14          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 2        | 0.14          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 2        | 0.14          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 2        | 0.14          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 17       | 0.14          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 17       | 0.14          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 17       | 0.14          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 12       | 0.14          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 12       | 0.14          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 12       | 0.14          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 13       | 0.14          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 13       | 0.14          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 13       | 0.14          |
| (1,460) | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD21 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD22 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD11 | 1:36:A:LEU:HD23 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD21 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD22 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD12 | 1:36:A:LEU:HD23 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD21 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD22 | 12       | 0.14          |
| (1,460) | 1:28:A:LEU:HD13 | 1:36:A:LEU:HD23 | 12       | 0.14          |
| (1,454) | 1:30:A:LYS:HD3  | 1:65:A:GLY:HA2  | 1        | 0.14          |
| (1,454) | 1:30:A:LYS:HD3  | 1:65:A:GLY:HA2  | 13       | 0.14          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 9        | 0.14          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 9        | 0.14          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 9        | 0.14          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 20       | 0.14          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 20       | 0.14          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 20       | 0.14          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 7        | 0.14          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 7        | 0.14          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 7        | 0.14          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 3        | 0.14          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 3        | 0.14          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 3        | 0.14          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 6        | 0.14          |
| (1,395) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 8        | 0.14          |
| (1,387) | 1:60:A:GLU:HA   | 1:60:A:GLU:HG3  | 6        | 0.14          |
| (1,387) | 1:60:A:GLU:HA   | 1:60:A:GLU:HG3  | 7        | 0.14          |
| (1,385) | 1:29:A:SER:HB2  | 1:31:A:LYS:HD2  | 16       | 0.14          |
| (1,362) | 1:73:A:GLU:HA   | 1:73:A:GLU:HG3  | 19       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,339) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HD2  | 6        | 0.14          |
| (1,339) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HD2  | 6        | 0.14          |
| (1,339) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HD2  | 6        | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 9        | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 14       | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 16       | 0.14          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 3        | 0.14          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 16       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 16       | 0.14          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 11       | 0.14          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 16       | 0.14          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 16       | 0.14          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 16       | 0.14          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 16       | 0.14          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 16       | 0.14          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 17       | 0.14          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 17       | 0.14          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 17       | 0.14          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 15       | 0.14          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 15       | 0.14          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 15       | 0.14          |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB1  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB2  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB3  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB1  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB2  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB3  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB1  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB2  | 20       | 0.14          |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB3  | 20       | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2 | 6        | 0.14          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3 | 6        | 0.14          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2 | 13       | 0.14          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3 | 13       | 0.14          |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2 | 11       | 0.14          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2 | 11       | 0.14          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2 | 11       | 0.14          |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2 | 16       | 0.14          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2 | 16       | 0.14          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2 | 16       | 0.14          |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2 | 18       | 0.14          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2 | 18       | 0.14          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2 | 18       | 0.14          |
| (1,259) | 1:37:A:LEU:HD21 | 1:41:A:LEU:HB2 | 14       | 0.14          |
| (1,259) | 1:37:A:LEU:HD22 | 1:41:A:LEU:HB2 | 14       | 0.14          |
| (1,259) | 1:37:A:LEU:HD23 | 1:41:A:LEU:HB2 | 14       | 0.14          |
| (1,250) | 1:86:A:ASN:HD22 | 1:9:B:GLU:HB2  | 18       | 0.14          |
| (1,241) | 1:86:A:ASN:HB3  | 1:12:B:ILE:HB  | 9        | 0.14          |
| (1,207) | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1 | 14       | 0.14          |
| (1,192) | 1:40:A:GLU:HG3  | 1:2:B:SER:HB3  | 5        | 0.14          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2 | 12       | 0.14          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2 | 18       | 0.14          |
| (1,166) | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2 | 19       | 0.14          |
| (1,166) | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2 | 19       | 0.14          |
| (1,166) | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2 | 19       | 0.14          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2 | 8        | 0.14          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2 | 8        | 0.14          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2 | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 9        | 0.14          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 9        | 0.14          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 9        | 0.14          |
| (1,151) | 1:80:A:ALA:HA   | 1:72:B:GLN:HA   | 12       | 0.14          |
| (1,144) | 1:11:A:LEU:HD11 | 1:4:B:LEU:HB2   | 11       | 0.14          |
| (1,144) | 1:11:A:LEU:HD12 | 1:4:B:LEU:HB2   | 11       | 0.14          |
| (1,144) | 1:11:A:LEU:HD13 | 1:4:B:LEU:HB2   | 11       | 0.14          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 7        | 0.14          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 13       | 0.14          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 13       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 4        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3 | 5        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3 | 6        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3 | 8        | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3 | 11       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3 | 18       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1 | 19       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2 | 19       | 0.14          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3 | 19       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1 | 19       | 0.14          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2 | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,104)  | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 19       | 0.14          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 19       | 0.14          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 19       | 0.14          |
| (1,104)  | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 19       | 0.14          |
| (1,81)   | 1:72:A:GLN:HA   | 1:80:B:ALA:HA   | 13       | 0.14          |
| (1,77)   | 1:4:A:LEU:HD21  | 1:13:B:ASN:HB2  | 17       | 0.14          |
| (1,77)   | 1:4:A:LEU:HD22  | 1:13:B:ASN:HB2  | 17       | 0.14          |
| (1,77)   | 1:4:A:LEU:HD23  | 1:13:B:ASN:HB2  | 17       | 0.14          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 11       | 0.14          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 11       | 0.14          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 11       | 0.14          |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 8        | 0.14          |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 15       | 0.14          |
| (1,47)   | 1:8:A:MET:HG3   | 1:41:B:LEU:HG   | 9        | 0.14          |
| (1,7)    | 1:8:A:MET:HE1   | 1:82:B:THR:H    | 4        | 0.14          |
| (1,7)    | 1:8:A:MET:HE2   | 1:82:B:THR:H    | 4        | 0.14          |
| (1,7)    | 1:8:A:MET:HE3   | 1:82:B:THR:H    | 4        | 0.14          |
| (1,3598) | 1:48:B:GLN:HE22 | 1:49:B:LYS:H    | 15       | 0.13          |
| (1,3586) | 1:43:B:GLY:H    | 1:46:B:ASP:HB2  | 10       | 0.13          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 5        | 0.13          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 5        | 0.13          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 5        | 0.13          |
| (1,3571) | 1:33:B:LEU:HB3  | 1:36:B:LEU:HG   | 1        | 0.13          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 7        | 0.13          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 14       | 0.13          |
| (1,3564) | 1:29:B:SER:HA   | 1:31:B:LYS:HE3  | 6        | 0.13          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 11       | 0.13          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 16       | 0.13          |
| (1,3553) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HE2  | 3        | 0.13          |
| (1,3552) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HE1  | 12       | 0.13          |
| (1,3549) | 1:20:B:GLY:HA3  | 1:21:B:LYS:HE2  | 14       | 0.13          |
| (1,3543) | 1:16:B:HIS:H    | 1:74:B:TYR:HE2  | 6        | 0.13          |
| (1,3543) | 1:16:B:HIS:H    | 1:74:B:TYR:HE2  | 10       | 0.13          |
| (1,3533) | 1:14:B:VAL:HA   | 1:74:B:TYR:HE2  | 17       | 0.13          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 5        | 0.13          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 8        | 0.13          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 12       | 0.13          |
| (1,3492) | 1:68:A:GLU:HB3  | 1:70:A:ASP:HB3  | 12       | 0.13          |
| (1,3477) | 1:51:A:VAL:HB   | 1:52:A:ASP:HB3  | 11       | 0.13          |
| (1,3463) | 1:47:A:ALA:H    | 1:48:A:GLN:HB3  | 18       | 0.13          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 9        | 0.13          |
| (1,3427) | 1:27:A:LYS:HE2  | 1:69:A:VAL:H    | 12       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3424) | 1:25:A:LYS:HG2  | 1:26:A:TYR:HE1  | 19       | 0.13          |
| (1,3415) | 1:16:A:HIS:H    | 1:74:A:TYR:HE2  | 8        | 0.13          |
| (1,3282) | 1:90:B:TRP:HE1  | 1:91:B:GLU:H    | 6        | 0.13          |
| (1,3275) | 1:26:A:TYR:HA   | 1:27:A:LYS:HD2  | 17       | 0.13          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 11       | 0.13          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 14       | 0.13          |
| (1,3201) | 1:45:A:LEU:HD11 | 1:46:A:ASP:HB3  | 14       | 0.13          |
| (1,3201) | 1:45:A:LEU:HD12 | 1:46:A:ASP:HB3  | 14       | 0.13          |
| (1,3201) | 1:45:A:LEU:HD13 | 1:46:A:ASP:HB3  | 14       | 0.13          |
| (1,3141) | 1:57:B:VAL:H    | 1:58:B:MET:HB3  | 10       | 0.13          |
| (1,2881) | 1:46:A:ASP:HB2  | 1:49:A:LYS:HG3  | 17       | 0.13          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 3        | 0.13          |
| (1,2601) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HD3  | 6        | 0.13          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 2        | 0.13          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 5        | 0.13          |
| (1,2370) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG2  | 5        | 0.13          |
| (1,2364) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG2  | 11       | 0.13          |
| (1,2364) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG2  | 20       | 0.13          |
| (1,2329) | 1:15:B:PHE:HD1  | 1:74:B:TYR:HB3  | 20       | 0.13          |
| (1,2261) | 1:39:A:THR:HG21 | 1:40:A:GLU:H    | 15       | 0.13          |
| (1,2261) | 1:39:A:THR:HG22 | 1:40:A:GLU:H    | 15       | 0.13          |
| (1,2261) | 1:39:A:THR:HG23 | 1:40:A:GLU:H    | 15       | 0.13          |
| (1,2044) | 1:63:A:GLU:HB2  | 1:64:A:ASN:H    | 15       | 0.13          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD21  | 3        | 0.13          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD22  | 3        | 0.13          |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD23  | 3        | 0.13          |
| (1,1675) | 1:55:A:ASP:HB3  | 1:56:A:LYS:HD2  | 15       | 0.13          |
| (1,1669) | 1:30:A:LYS:HA   | 1:33:A:LEU:HB3  | 19       | 0.13          |
| (1,1628) | 1:27:A:LYS:HE3  | 1:68:A:GLU:HB3  | 7        | 0.13          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 19       | 0.13          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 19       | 0.13          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 19       | 0.13          |
| (1,1611) | 1:27:B:LYS:HD2  | 1:70:B:ASP:HB3  | 13       | 0.13          |
| (1,1606) | 1:83:B:VAL:HG11 | 1:84:B:ALA:H    | 2        | 0.13          |
| (1,1606) | 1:83:B:VAL:HG12 | 1:84:B:ALA:H    | 2        | 0.13          |
| (1,1606) | 1:83:B:VAL:HG13 | 1:84:B:ALA:H    | 2        | 0.13          |
| (1,1606) | 1:83:B:VAL:HG11 | 1:84:B:ALA:H    | 19       | 0.13          |
| (1,1606) | 1:83:B:VAL:HG12 | 1:84:B:ALA:H    | 19       | 0.13          |
| (1,1606) | 1:83:B:VAL:HG13 | 1:84:B:ALA:H    | 19       | 0.13          |
| (1,1594) | 1:41:B:LEU:HB2  | 1:45:B:LEU:HB3  | 17       | 0.13          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD21  | 7        | 0.13          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD22  | 7        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD23  | 7        | 0.13          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 3        | 0.13          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 3        | 0.13          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 3        | 0.13          |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 8        | 0.13          |
| (1,1452) | 1:22:A:GLU:HB2  | 1:31:A:LYS:HG2  | 9        | 0.13          |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD21 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD22 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD23 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD21 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD22 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD23 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD21 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD22 | 18       | 0.13          |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD23 | 18       | 0.13          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD21 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD22 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD23 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD21 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD22 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD23 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD21 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD22 | 8        | 0.13          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD23 | 8        | 0.13          |
| (1,1359) | 1:36:B:LEU:HD11 | 1:40:B:GLU:HG3  | 18       | 0.13          |
| (1,1359) | 1:36:B:LEU:HD12 | 1:40:B:GLU:HG3  | 18       | 0.13          |
| (1,1359) | 1:36:B:LEU:HD13 | 1:40:B:GLU:HG3  | 18       | 0.13          |
| (1,1354) | 1:36:A:LEU:HD11 | 1:40:A:GLU:HG3  | 12       | 0.13          |
| (1,1354) | 1:36:A:LEU:HD12 | 1:40:A:GLU:HG3  | 12       | 0.13          |
| (1,1354) | 1:36:A:LEU:HD13 | 1:40:A:GLU:HG3  | 12       | 0.13          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 19       | 0.13          |
| (1,1325) | 1:58:A:MET:HA   | 1:61:A:LEU:HD21 | 8        | 0.13          |
| (1,1325) | 1:58:A:MET:HA   | 1:61:A:LEU:HD22 | 8        | 0.13          |
| (1,1325) | 1:58:A:MET:HA   | 1:61:A:LEU:HD23 | 8        | 0.13          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 8        | 0.13          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 18       | 0.13          |
| (1,1257) | 1:38:A:GLN:HG3  | 1:39:A:THR:HG21 | 9        | 0.13          |
| (1,1257) | 1:38:A:GLN:HG3  | 1:39:A:THR:HG22 | 9        | 0.13          |
| (1,1257) | 1:38:A:GLN:HG3  | 1:39:A:THR:HG23 | 9        | 0.13          |
| (1,1234) | 1:91:B:GLU:H    | 1:91:B:GLU:HG2  | 12       | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 3        | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 3        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 3        | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 9        | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 9        | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 9        | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 12       | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 12       | 0.13          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 12       | 0.13          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 2        | 0.13          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 2        | 0.13          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 2        | 0.13          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 12       | 0.13          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 12       | 0.13          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 12       | 0.13          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE1  | 4        | 0.13          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE2  | 4        | 0.13          |
| (1,1144) | 1:44:A:PHE:HE2  | 1:85:A:MET:HE3  | 4        | 0.13          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 17       | 0.13          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 17       | 0.13          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 17       | 0.13          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 5        | 0.13          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 5        | 0.13          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 5        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 2        | 0.13          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 13       | 0.13          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 13       | 0.13          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 1        | 0.13          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 1        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 1        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 1        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 1        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 1        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 1        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 1        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 1        | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 2        | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 6        | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 11       | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 14       | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 14       | 0.13          |
| (1,988) | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 14       | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 14       | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 14       | 0.13          |
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 14       | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 14       | 0.13          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 14       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 14       | 0.13          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 6        | 0.13          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 6        | 0.13          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 6        | 0.13          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 12       | 0.13          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 12       | 0.13          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 12       | 0.13          |
| (1,963) | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 6        | 0.13          |
| (1,962) | 1:27:B:LYS:HA   | 1:27:B:LYS:HD2  | 7        | 0.13          |
| (1,962) | 1:27:B:LYS:HA   | 1:27:B:LYS:HD2  | 10       | 0.13          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 1        | 0.13          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 1        | 0.13          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 1        | 0.13          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 9        | 0.13          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 9        | 0.13          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 9        | 0.13          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 10       | 0.13          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 10       | 0.13          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 10       | 0.13          |
| (1,952) | 1:29:A:SER:HB3  | 1:68:A:GLU:HG3  | 7        | 0.13          |
| (1,952) | 1:29:A:SER:HB3  | 1:68:A:GLU:HG3  | 10       | 0.13          |
| (1,951) | 1:27:A:LYS:HA   | 1:27:A:LYS:HD2  | 18       | 0.13          |
| (1,928) | 1:31:B:LYS:H    | 1:31:B:LYS:HG2  | 18       | 0.13          |
| (1,920) | 1:38:A:GLN:HG3  | 1:39:A:THR:HB   | 2        | 0.13          |
| (1,918) | 1:31:A:LYS:H    | 1:31:A:LYS:HG2  | 7        | 0.13          |
| (1,852) | 1:89:A:PHE:HB3  | 1:90:A:TRP:HD1  | 2        | 0.13          |
| (1,839) | 1:38:B:GLN:HA   | 1:45:B:LEU:HD21 | 3        | 0.13          |
| (1,839) | 1:38:B:GLN:HA   | 1:45:B:LEU:HD22 | 3        | 0.13          |
| (1,839) | 1:38:B:GLN:HA   | 1:45:B:LEU:HD23 | 3        | 0.13          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD11 | 11       | 0.13          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD12 | 11       | 0.13          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD13 | 11       | 0.13          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD11 | 14       | 0.13          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD12 | 14       | 0.13          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD13 | 14       | 0.13          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD11 | 15       | 0.13          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD12 | 15       | 0.13          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD13 | 15       | 0.13          |
| (1,655) | 1:30:A:LYS:HE3  | 1:69:A:VAL:HG21 | 6        | 0.13          |
| (1,655) | 1:30:A:LYS:HE3  | 1:69:A:VAL:HG22 | 6        | 0.13          |
| (1,655) | 1:30:A:LYS:HE3  | 1:69:A:VAL:HG23 | 6        | 0.13          |
| (1,621) | 1:9:A:GLU:HA    | 1:12:A:ILE:HB   | 5        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,621) | 1:9:A:GLU:HA    | 1:12:A:ILE:HB   | 19       | 0.13          |
| (1,572) | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 13       | 0.13          |
| (1,572) | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 13       | 0.13          |
| (1,572) | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 13       | 0.13          |
| (1,572) | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 18       | 0.13          |
| (1,572) | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 18       | 0.13          |
| (1,572) | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 18       | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 2        | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 2        | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 2        | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 10       | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 10       | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 10       | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG21 | 11       | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG22 | 11       | 0.13          |
| (1,559) | 1:36:A:LEU:HA   | 1:39:A:THR:HG23 | 11       | 0.13          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG11 | 19       | 0.13          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG12 | 19       | 0.13          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG13 | 19       | 0.13          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 11       | 0.13          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 11       | 0.13          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 11       | 0.13          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 13       | 0.13          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 13       | 0.13          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 13       | 0.13          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE2  | 6        | 0.13          |
| (1,522) | 1:59:A:LYS:HB2  | 1:59:A:LYS:HE3  | 6        | 0.13          |
| (1,513) | 1:14:B:VAL:H    | 1:14:B:VAL:HG21 | 9        | 0.13          |
| (1,513) | 1:14:B:VAL:H    | 1:14:B:VAL:HG22 | 9        | 0.13          |
| (1,513) | 1:14:B:VAL:H    | 1:14:B:VAL:HG23 | 9        | 0.13          |
| (1,499) | 1:57:A:VAL:HG21 | 1:81:A:LEU:HG   | 9        | 0.13          |
| (1,499) | 1:57:A:VAL:HG22 | 1:81:A:LEU:HG   | 9        | 0.13          |
| (1,499) | 1:57:A:VAL:HG23 | 1:81:A:LEU:HG   | 9        | 0.13          |
| (1,482) | 1:89:B:PHE:HA   | 1:89:B:PHE:HD1  | 10       | 0.13          |
| (1,457) | 1:30:B:LYS:HD3  | 1:65:B:GLY:HA2  | 5        | 0.13          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 12       | 0.13          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 12       | 0.13          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 12       | 0.13          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 18       | 0.13          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 18       | 0.13          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 18       | 0.13          |
| (1,429) | 1:26:A:TYR:HB2  | 1:26:A:TYR:HD2  | 8        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG21 | 14       | 0.13          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG22 | 14       | 0.13          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG23 | 14       | 0.13          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG21 | 19       | 0.13          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG22 | 19       | 0.13          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG23 | 19       | 0.13          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 1        | 0.13          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 4        | 0.13          |
| (1,391) | 1:60:B:GLU:HA   | 1:60:B:GLU:HG3  | 4        | 0.13          |
| (1,390) | 1:30:B:LYS:HG3  | 1:65:B:GLY:HA3  | 15       | 0.13          |
| (1,386) | 1:30:A:LYS:HG3  | 1:65:A:GLY:HA3  | 12       | 0.13          |
| (1,364) | 1:73:B:GLU:HA   | 1:73:B:GLU:HG3  | 9        | 0.13          |
| (1,339) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HD2  | 5        | 0.13          |
| (1,339) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HD2  | 5        | 0.13          |
| (1,339) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HD2  | 5        | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 7        | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 18       | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 20       | 0.13          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 20       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 5        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 6        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 7        | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 11       | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 18       | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 18       | 0.13          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 18       | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 18       | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 18       | 0.13          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 18       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 18       | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 18       | 0.13          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 18       | 0.13          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD11 | 15       | 0.13          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD12 | 15       | 0.13          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD13 | 15       | 0.13          |
| (1,294) | 1:77:A:LEU:HA   | 1:77:A:LEU:HD11 | 11       | 0.13          |
| (1,294) | 1:77:A:LEU:HA   | 1:77:A:LEU:HD12 | 11       | 0.13          |
| (1,294) | 1:77:A:LEU:HA   | 1:77:A:LEU:HD13 | 11       | 0.13          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 1        | 0.13          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 1        | 0.13          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 1        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 1        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 1        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 1        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 5        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 5        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 5        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 6        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 6        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 6        | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 10       | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 10       | 0.13          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 10       | 0.13          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 3        | 0.13          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 3        | 0.13          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 7        | 0.13          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 7        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2  | 7        | 0.13          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2  | 7        | 0.13          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2  | 7        | 0.13          |
| (1,242) | 1:86:A:ASN:HB3  | 1:12:B:ILE:HA   | 12       | 0.13          |
| (1,242) | 1:86:A:ASN:HB3  | 1:12:B:ILE:HA   | 16       | 0.13          |
| (1,202) | 1:43:A:GLY:H    | 1:1:B:GLY:HA2   | 9        | 0.13          |
| (1,202) | 1:43:A:GLY:H    | 1:1:B:GLY:HA3   | 9        | 0.13          |
| (1,184) | 1:41:A:LEU:HA   | 1:5:B:GLU:HG2   | 5        | 0.13          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 17       | 0.13          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 14       | 0.13          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 14       | 0.13          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 14       | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 2        | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 15       | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 20       | 0.13          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 20       | 0.13          |
| (1,129) | 1:11:A:LEU:HD21 | 1:7:B:ALA:H     | 10       | 0.13          |
| (1,129) | 1:11:A:LEU:HD22 | 1:7:B:ALA:H     | 10       | 0.13          |
| (1,129) | 1:11:A:LEU:HD23 | 1:7:B:ALA:H     | 10       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 14       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 15       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 16       | 0.13          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 16       | 0.13          |
| (1,99)  | 1:7:A:ALA:HB1   | 1:11:B:LEU:HG   | 17       | 0.13          |
| (1,99)  | 1:7:A:ALA:HB2   | 1:11:B:LEU:HG   | 17       | 0.13          |
| (1,99)  | 1:7:A:ALA:HB3   | 1:11:B:LEU:HG   | 17       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG21 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG22 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG23 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG21 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG22 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG23 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG21 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG22 | 16       | 0.13          |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG23 | 16       | 0.13          |
| (1,67)  | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 1        | 0.13          |
| (1,67)  | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 1        | 0.13          |
| (1,67)  | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 1        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 11       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 11       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 11       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 13       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 13       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 13       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG21 | 19       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG22 | 19       | 0.13          |
| (1,67)   | 1:72:A:GLN:HB2  | 1:83:B:VAL:HG23 | 19       | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 7        | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 7        | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 7        | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 8        | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 8        | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 8        | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG11 | 13       | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG12 | 13       | 0.13          |
| (1,60)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HG13 | 13       | 0.13          |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 5        | 0.13          |
| (1,56)   | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 10       | 0.13          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 8        | 0.12          |
| (1,3611) | 1:57:B:VAL:HB   | 1:77:B:LEU:HG   | 14       | 0.12          |
| (1,3605) | 1:51:B:VAL:HB   | 1:52:B:ASP:HB3  | 7        | 0.12          |
| (1,3598) | 1:48:B:GLN:HE22 | 1:49:B:LYS:H    | 19       | 0.12          |
| (1,3576) | 1:37:B:LEU:HD21 | 1:44:B:PHE:HD1  | 11       | 0.12          |
| (1,3576) | 1:37:B:LEU:HD22 | 1:44:B:PHE:HD1  | 11       | 0.12          |
| (1,3576) | 1:37:B:LEU:HD23 | 1:44:B:PHE:HD1  | 11       | 0.12          |
| (1,3575) | 1:37:B:LEU:HB2  | 1:74:B:TYR:HA   | 3        | 0.12          |
| (1,3567) | 1:31:B:LYS:HE2  | 1:32:B:GLU:H    | 12       | 0.12          |
| (1,3556) | 1:27:B:LYS:HE3  | 1:69:B:VAL:H    | 8        | 0.12          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 1        | 0.12          |
| (1,3533) | 1:14:B:VAL:HA   | 1:74:B:TYR:HE2  | 8        | 0.12          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 1        | 0.12          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 20       | 0.12          |
| (1,3522) | 1:6:B:THR:HG21  | 1:9:B:GLU:HA    | 6        | 0.12          |
| (1,3522) | 1:6:B:THR:HG22  | 1:9:B:GLU:HA    | 6        | 0.12          |
| (1,3522) | 1:6:B:THR:HG23  | 1:9:B:GLU:HA    | 6        | 0.12          |
| (1,3522) | 1:6:B:THR:HG21  | 1:9:B:GLU:HA    | 9        | 0.12          |
| (1,3522) | 1:6:B:THR:HG22  | 1:9:B:GLU:HA    | 9        | 0.12          |
| (1,3522) | 1:6:B:THR:HG23  | 1:9:B:GLU:HA    | 9        | 0.12          |
| (1,3522) | 1:6:B:THR:HG21  | 1:9:B:GLU:HA    | 15       | 0.12          |
| (1,3522) | 1:6:B:THR:HG22  | 1:9:B:GLU:HA    | 15       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3522) | 1:6:B:THR:HG23  | 1:9:B:GLU:HA    | 15       | 0.12          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 13       | 0.12          |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 16       | 0.12          |
| (1,3483) | 1:57:A:VAL:HB   | 1:77:A:LEU:HG   | 19       | 0.12          |
| (1,3472) | 1:49:A:LYS:H    | 1:54:A:VAL:HB   | 20       | 0.12          |
| (1,3463) | 1:47:A:ALA:H    | 1:48:A:GLN:HB3  | 19       | 0.12          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 19       | 0.12          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 19       | 0.12          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 19       | 0.12          |
| (1,3443) | 1:33:A:LEU:HB3  | 1:36:A:LEU:HG   | 2        | 0.12          |
| (1,3432) | 1:28:A:LEU:HD21 | 1:35:A:GLU:H    | 8        | 0.12          |
| (1,3432) | 1:28:A:LEU:HD22 | 1:35:A:GLU:H    | 8        | 0.12          |
| (1,3432) | 1:28:A:LEU:HD23 | 1:35:A:GLU:H    | 8        | 0.12          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 15       | 0.12          |
| (1,3415) | 1:16:A:HIS:H    | 1:74:A:TYR:HE2  | 9        | 0.12          |
| (1,3415) | 1:16:A:HIS:H    | 1:74:A:TYR:HE2  | 20       | 0.12          |
| (1,3400) | 1:9:A:GLU:HA    | 1:71:A:PHE:HE2  | 11       | 0.12          |
| (1,3393) | 1:1:A:GLY:HA2   | 1:5:A:GLU:HG2   | 17       | 0.12          |
| (1,3388) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HE2  | 4        | 0.12          |
| (1,3385) | 1:66:A:ASP:HB2  | 1:68:A:GLU:H    | 14       | 0.12          |
| (1,3382) | 1:37:A:LEU:HA   | 1:40:A:GLU:HG3  | 8        | 0.12          |
| (1,3181) | 1:27:B:LYS:HE3  | 1:71:B:PHE:H    | 9        | 0.12          |
| (1,3170) | 1:48:B:GLN:H    | 1:54:B:VAL:HB   | 15       | 0.12          |
| (1,3133) | 1:57:A:VAL:H    | 1:58:A:MET:HB3  | 8        | 0.12          |
| (1,3105) | 1:15:B:PHE:HE1  | 1:70:B:ASP:HB3  | 20       | 0.12          |
| (1,3034) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HE1  | 12       | 0.12          |
| (1,3034) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HE1  | 12       | 0.12          |
| (1,3034) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HE1  | 12       | 0.12          |
| (1,2917) | 1:19:B:SER:HB2  | 1:28:B:LEU:HB2  | 9        | 0.12          |
| (1,2889) | 1:14:A:VAL:HA   | 1:40:A:GLU:HG3  | 20       | 0.12          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 4        | 0.12          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 6        | 0.12          |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 19       | 0.12          |
| (1,2838) | 1:91:A:GLU:HB2  | 1:93:A:SER:HB2  | 10       | 0.12          |
| (1,2522) | 1:15:A:PHE:HE1  | 1:74:A:TYR:HB3  | 12       | 0.12          |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 12       | 0.12          |
| (1,2472) | 1:59:A:LYS:HG3  | 1:60:A:GLU:HB2  | 2        | 0.12          |
| (1,2472) | 1:59:A:LYS:HG3  | 1:60:A:GLU:HB2  | 16       | 0.12          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 11       | 0.12          |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 3        | 0.12          |
| (1,2395) | 1:1:A:GLY:HA2   | 1:5:A:GLU:HB3   | 15       | 0.12          |
| (1,2364) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG2  | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2364) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG2  | 18       | 0.12          |
| (1,2239) | 1:30:B:LYS:H    | 1:30:B:LYS:HG2  | 12       | 0.12          |
| (1,2148) | 1:25:B:LYS:HE3  | 1:26:B:TYR:HD1  | 15       | 0.12          |
| (1,2103) | 1:63:A:GLU:HB2  | 1:64:A:ASN:HD21 | 9        | 0.12          |
| (1,2100) | 1:25:A:LYS:HG3  | 1:26:A:TYR:HA   | 3        | 0.12          |
| (1,2082) | 1:25:B:LYS:HG3  | 1:26:B:TYR:H    | 3        | 0.12          |
| (1,2082) | 1:25:B:LYS:HG3  | 1:26:B:TYR:H    | 9        | 0.12          |
| (1,1734) | 1:54:A:VAL:HG21 | 1:55:A:ASP:H    | 17       | 0.12          |
| (1,1734) | 1:54:A:VAL:HG22 | 1:55:A:ASP:H    | 17       | 0.12          |
| (1,1734) | 1:54:A:VAL:HG23 | 1:55:A:ASP:H    | 17       | 0.12          |
| (1,1678) | 1:30:B:LYS:HA   | 1:33:B:LEU:HB3  | 18       | 0.12          |
| (1,1669) | 1:30:A:LYS:HA   | 1:33:A:LEU:HB3  | 18       | 0.12          |
| (1,1643) | 1:52:B:ASP:HB3  | 1:53:B:ALA:HB1  | 10       | 0.12          |
| (1,1643) | 1:52:B:ASP:HB3  | 1:53:B:ALA:HB2  | 10       | 0.12          |
| (1,1643) | 1:52:B:ASP:HB3  | 1:53:B:ALA:HB3  | 10       | 0.12          |
| (1,1623) | 1:30:B:LYS:HE2  | 1:33:B:LEU:HB3  | 16       | 0.12          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 2        | 0.12          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 2        | 0.12          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 2        | 0.12          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 20       | 0.12          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 20       | 0.12          |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 20       | 0.12          |
| (1,1616) | 1:30:A:LYS:HE2  | 1:33:A:LEU:HB3  | 14       | 0.12          |
| (1,1616) | 1:30:A:LYS:HE2  | 1:33:A:LEU:HB3  | 17       | 0.12          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG11 | 4        | 0.12          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG12 | 4        | 0.12          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG13 | 4        | 0.12          |
| (1,1593) | 1:25:B:LYS:HB2  | 1:25:B:LYS:HE3  | 3        | 0.12          |
| (1,1593) | 1:25:B:LYS:HB2  | 1:25:B:LYS:HE3  | 13       | 0.12          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 3        | 0.12          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 14       | 0.12          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 19       | 0.12          |
| (1,1456) | 1:22:B:GLU:HB2  | 1:31:B:LYS:HG2  | 12       | 0.12          |
| (1,1395) | 1:31:B:LYS:HB2  | 1:32:B:GLU:H    | 2        | 0.12          |
| (1,1358) | 1:27:B:LYS:HB3  | 1:68:B:GLU:HB3  | 12       | 0.12          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 3        | 0.12          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 7        | 0.12          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 13       | 0.12          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 10       | 0.12          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 14       | 0.12          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 20       | 0.12          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 16       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 16       | 0.12          |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 16       | 0.12          |
| (1,1230) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HB2  | 6        | 0.12          |
| (1,1230) | 1:41:B:LEU:HB3  | 1:44:B:PHE:HB2  | 16       | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 9        | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 9        | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 9        | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 14       | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 14       | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 14       | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 20       | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 20       | 0.12          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 20       | 0.12          |
| (1,1221) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HB2  | 15       | 0.12          |
| (1,1204) | 1:88:A:PHE:HD1  | 1:85:A:MET:HG2  | 6        | 0.12          |
| (1,1204) | 1:88:A:PHE:HD1  | 1:85:A:MET:HG3  | 6        | 0.12          |
| (1,1204) | 1:88:A:PHE:HD2  | 1:85:A:MET:HG2  | 6        | 0.12          |
| (1,1204) | 1:88:A:PHE:HD2  | 1:85:A:MET:HG3  | 6        | 0.12          |
| (1,1203) | 1:88:A:PHE:HD1  | 1:85:A:MET:HG2  | 6        | 0.12          |
| (1,1203) | 1:88:A:PHE:HD1  | 1:85:A:MET:HG3  | 6        | 0.12          |
| (1,1203) | 1:88:A:PHE:HD2  | 1:85:A:MET:HG2  | 6        | 0.12          |
| (1,1203) | 1:88:A:PHE:HD2  | 1:85:A:MET:HG3  | 6        | 0.12          |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 16       | 0.12          |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 16       | 0.12          |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 16       | 0.12          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 4        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 4        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 4        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 7        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 7        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 7        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 8        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 8        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 8        | 0.12          |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 13       | 0.12          |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 13       | 0.12          |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 13       | 0.12          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 7        | 0.12          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 7        | 0.12          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 7        | 0.12          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 7        | 0.12          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 7        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 7        | 0.12          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 7        | 0.12          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 7        | 0.12          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 7        | 0.12          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 5        | 0.12          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 5        | 0.12          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 5        | 0.12          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 17       | 0.12          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 17       | 0.12          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 17       | 0.12          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 20       | 0.12          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 20       | 0.12          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 20       | 0.12          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 3        | 0.12          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 3        | 0.12          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 3        | 0.12          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 16       | 0.12          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 16       | 0.12          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 16       | 0.12          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD21 | 9        | 0.12          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD22 | 9        | 0.12          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD23 | 9        | 0.12          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD21 | 19       | 0.12          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD22 | 19       | 0.12          |
| (1,832) | 1:38:A:GLN:HA   | 1:45:A:LEU:HD23 | 19       | 0.12          |
| (1,751) | 1:51:B:VAL:HG11 | 1:53:B:ALA:H    | 20       | 0.12          |
| (1,751) | 1:51:B:VAL:HG12 | 1:53:B:ALA:H    | 20       | 0.12          |
| (1,751) | 1:51:B:VAL:HG13 | 1:53:B:ALA:H    | 20       | 0.12          |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD11 | 7        | 0.12          |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD12 | 7        | 0.12          |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD13 | 7        | 0.12          |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD11 | 20       | 0.12          |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD12 | 20       | 0.12          |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD13 | 20       | 0.12          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD11 | 16       | 0.12          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD12 | 16       | 0.12          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD13 | 16       | 0.12          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD11 | 8        | 0.12          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD12 | 8        | 0.12          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD13 | 8        | 0.12          |
| (1,715) | 1:69:A:VAL:H    | 1:69:A:VAL:HG11 | 3        | 0.12          |
| (1,715) | 1:69:A:VAL:H    | 1:69:A:VAL:HG12 | 3        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,715) | 1:69:A:VAL:H    | 1:69:A:VAL:HG13 | 3        | 0.12          |
| (1,678) | 1:57:A:VAL:HG11 | 1:81:A:LEU:HG   | 14       | 0.12          |
| (1,678) | 1:57:A:VAL:HG12 | 1:81:A:LEU:HG   | 14       | 0.12          |
| (1,678) | 1:57:A:VAL:HG13 | 1:81:A:LEU:HG   | 14       | 0.12          |
| (1,600) | 1:83:B:VAL:H    | 1:83:B:VAL:HG11 | 1        | 0.12          |
| (1,600) | 1:83:B:VAL:H    | 1:83:B:VAL:HG12 | 1        | 0.12          |
| (1,600) | 1:83:B:VAL:H    | 1:83:B:VAL:HG13 | 1        | 0.12          |
| (1,572) | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 10       | 0.12          |
| (1,572) | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 10       | 0.12          |
| (1,572) | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 10       | 0.12          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG11 | 4        | 0.12          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG12 | 4        | 0.12          |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG13 | 4        | 0.12          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE1  | 16       | 0.12          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE2  | 16       | 0.12          |
| (1,538) | 1:55:B:ASP:HA   | 1:58:B:MET:HE3  | 16       | 0.12          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 4        | 0.12          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 4        | 0.12          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 4        | 0.12          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 16       | 0.12          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 16       | 0.12          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 16       | 0.12          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 9        | 0.12          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 9        | 0.12          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 9        | 0.12          |
| (1,406) | 1:72:A:GLN:HA   | 1:75:A:VAL:HG21 | 13       | 0.12          |
| (1,406) | 1:72:A:GLN:HA   | 1:75:A:VAL:HG22 | 13       | 0.12          |
| (1,406) | 1:72:A:GLN:HA   | 1:75:A:VAL:HG23 | 13       | 0.12          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 11       | 0.12          |
| (1,399) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG2  | 18       | 0.12          |
| (1,395) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 20       | 0.12          |
| (1,339) | 1:12:A:ILE:HG21 | 1:16:A:HIS:HD2  | 18       | 0.12          |
| (1,339) | 1:12:A:ILE:HG22 | 1:16:A:HIS:HD2  | 18       | 0.12          |
| (1,339) | 1:12:A:ILE:HG23 | 1:16:A:HIS:HD2  | 18       | 0.12          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 1        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 1        | 0.12          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 2        | 0.12          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 2        | 0.12          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 12       | 0.12          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 12       | 0.12          |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 12       | 0.12          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 4        | 0.12          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD21 | 18       | 0.12          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD22 | 18       | 0.12          |
| (1,327) | 1:28:A:LEU:HD21 | 1:36:A:LEU:HD23 | 18       | 0.12          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD21 | 18       | 0.12          |
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD22 | 18       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,327) | 1:28:A:LEU:HD22 | 1:36:A:LEU:HD23 | 18       | 0.12          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD21 | 18       | 0.12          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD22 | 18       | 0.12          |
| (1,327) | 1:28:A:LEU:HD23 | 1:36:A:LEU:HD23 | 18       | 0.12          |
| (1,314) | 1:56:B:LYS:HB2  | 1:56:B:LYS:HD2  | 1        | 0.12          |
| (1,314) | 1:56:B:LYS:HB2  | 1:56:B:LYS:HD2  | 3        | 0.12          |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD21 | 7        | 0.12          |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD22 | 7        | 0.12          |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD23 | 7        | 0.12          |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD21 | 17       | 0.12          |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD22 | 17       | 0.12          |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD23 | 17       | 0.12          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD11 | 11       | 0.12          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD12 | 11       | 0.12          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD13 | 11       | 0.12          |
| (1,287) | 1:61:A:LEU:HA   | 1:61:A:LEU:HD21 | 5        | 0.12          |
| (1,287) | 1:61:A:LEU:HA   | 1:61:A:LEU:HD22 | 5        | 0.12          |
| (1,287) | 1:61:A:LEU:HA   | 1:61:A:LEU:HD23 | 5        | 0.12          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 8        | 0.12          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 8        | 0.12          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 8        | 0.12          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2  | 20       | 0.12          |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3  | 20       | 0.12          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2  | 8        | 0.12          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3  | 8        | 0.12          |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2  | 12       | 0.12          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2  | 12       | 0.12          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2  | 12       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,241) | 1:86:A:ASN:HB3  | 1:12:B:ILE:HB   | 4        | 0.12          |
| (1,235) | 1:82:A:THR:H    | 1:8:B:MET:HE1   | 17       | 0.12          |
| (1,235) | 1:82:A:THR:H    | 1:8:B:MET:HE2   | 17       | 0.12          |
| (1,235) | 1:82:A:THR:H    | 1:8:B:MET:HE3   | 17       | 0.12          |
| (1,194) | 1:40:A:GLU:HB3  | 1:2:B:SER:HB3   | 1        | 0.12          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 5        | 0.12          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 13       | 0.12          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2  | 16       | 0.12          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 5        | 0.12          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 5        | 0.12          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 5        | 0.12          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 11       | 0.12          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 11       | 0.12          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 11       | 0.12          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 17       | 0.12          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 17       | 0.12          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 17       | 0.12          |
| (1,144) | 1:11:A:LEU:HD11 | 1:4:B:LEU:HB2   | 16       | 0.12          |
| (1,144) | 1:11:A:LEU:HD12 | 1:4:B:LEU:HB2   | 16       | 0.12          |
| (1,144) | 1:11:A:LEU:HD13 | 1:4:B:LEU:HB2   | 16       | 0.12          |
| (1,139) | 1:80:A:ALA:HA   | 1:75:B:VAL:HG11 | 8        | 0.12          |
| (1,139) | 1:80:A:ALA:HA   | 1:75:B:VAL:HG12 | 8        | 0.12          |
| (1,139) | 1:80:A:ALA:HA   | 1:75:B:VAL:HG13 | 8        | 0.12          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 4        | 0.12          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 12       | 0.12          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 12       | 0.12          |
| (1,129) | 1:11:A:LEU:HD21 | 1:7:B:ALA:H     | 14       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,129) | 1:11:A:LEU:HD22 | 1:7:B:ALA:H     | 14       | 0.12          |
| (1,129) | 1:11:A:LEU:HD23 | 1:7:B:ALA:H     | 14       | 0.12          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 17       | 0.12          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 20       | 0.12          |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 20       | 0.12          |
| (1,95)  | 1:75:A:VAL:HG21 | 1:80:B:ALA:HA   | 8        | 0.12          |
| (1,95)  | 1:75:A:VAL:HG22 | 1:80:B:ALA:HA   | 8        | 0.12          |
| (1,95)  | 1:75:A:VAL:HG23 | 1:80:B:ALA:HA   | 8        | 0.12          |
| (1,85)  | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 2        | 0.12          |
| (1,85)  | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 4        | 0.12          |
| (1,81)  | 1:72:A:GLN:HA   | 1:80:B:ALA:HA   | 5        | 0.12          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG21 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG22 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG23 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG21 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG22 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG23 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG21 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG22 | 12       | 0.12          |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG23 | 12       | 0.12          |
| (1,56)  | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 4        | 0.12          |
| (1,56)  | 1:71:A:PHE:HD2  | 1:83:B:VAL:HB   | 17       | 0.12          |
| (1,39)  | 1:4:A:LEU:HD21  | 1:40:B:GLU:HA   | 18       | 0.12          |
| (1,39)  | 1:4:A:LEU:HD22  | 1:40:B:GLU:HA   | 18       | 0.12          |
| (1,39)  | 1:4:A:LEU:HD23  | 1:40:B:GLU:HA   | 18       | 0.12          |
| (1,32)  | 1:4:A:LEU:HB2   | 1:41:B:LEU:HA   | 17       | 0.12          |
| (1,10)  | 1:9:A:GLU:HA    | 1:82:B:THR:HG21 | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,10)   | 1:9:A:GLU:HA    | 1:82:B:THR:HG22 | 7        | 0.12          |
| (1,10)   | 1:9:A:GLU:HA    | 1:82:B:THR:HG23 | 7        | 0.12          |
| (1,7)    | 1:8:A:MET:HE1   | 1:82:B:THR:H    | 19       | 0.12          |
| (1,7)    | 1:8:A:MET:HE2   | 1:82:B:THR:H    | 19       | 0.12          |
| (1,7)    | 1:8:A:MET:HE3   | 1:82:B:THR:H    | 19       | 0.12          |
| (1,3619) | 1:64:B:ASN:HB3  | 1:67:B:GLY:H    | 13       | 0.11          |
| (1,3618) | 1:63:B:GLU:HG3  | 1:64:B:ASN:HB2  | 18       | 0.11          |
| (1,3617) | 1:63:B:GLU:HA   | 1:66:B:ASP:HB2  | 1        | 0.11          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD21 | 9        | 0.11          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD22 | 9        | 0.11          |
| (1,3572) | 1:34:B:LYS:HA   | 1:36:B:LEU:HD23 | 9        | 0.11          |
| (1,3568) | 1:31:B:LYS:HE2  | 1:32:B:GLU:HG2  | 8        | 0.11          |
| (1,3554) | 1:27:B:LYS:HB3  | 1:70:B:ASP:HB3  | 4        | 0.11          |
| (1,3552) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HE1  | 15       | 0.11          |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 15       | 0.11          |
| (1,3538) | 1:15:B:PHE:HE2  | 1:28:B:LEU:HD11 | 9        | 0.11          |
| (1,3538) | 1:15:B:PHE:HE2  | 1:28:B:LEU:HD12 | 9        | 0.11          |
| (1,3538) | 1:15:B:PHE:HE2  | 1:28:B:LEU:HD13 | 9        | 0.11          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 3        | 0.11          |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 10       | 0.11          |
| (1,3520) | 1:92:A:ASN:HB3  | 1:93:A:SER:HB2  | 15       | 0.11          |
| (1,3490) | 1:63:A:GLU:HG3  | 1:64:A:ASN:HB2  | 1        | 0.11          |
| (1,3489) | 1:63:A:GLU:HA   | 1:66:A:ASP:HB2  | 2        | 0.11          |
| (1,3489) | 1:63:A:GLU:HA   | 1:66:A:ASP:HB2  | 3        | 0.11          |
| (1,3486) | 1:58:A:MET:HG2  | 1:60:A:GLU:H    | 11       | 0.11          |
| (1,3477) | 1:51:A:VAL:HB   | 1:52:A:ASP:HB3  | 6        | 0.11          |
| (1,3472) | 1:49:A:LYS:H    | 1:54:A:VAL:HB   | 13       | 0.11          |
| (1,3448) | 1:37:A:LEU:HD21 | 1:44:A:PHE:HD1  | 14       | 0.11          |
| (1,3448) | 1:37:A:LEU:HD22 | 1:44:A:PHE:HD1  | 14       | 0.11          |
| (1,3448) | 1:37:A:LEU:HD23 | 1:44:A:PHE:HD1  | 14       | 0.11          |
| (1,3447) | 1:37:A:LEU:HB2  | 1:74:A:TYR:HA   | 18       | 0.11          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 9        | 0.11          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 9        | 0.11          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 9        | 0.11          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD21 | 12       | 0.11          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD22 | 12       | 0.11          |
| (1,3444) | 1:34:A:LYS:HA   | 1:36:A:LEU:HD23 | 12       | 0.11          |
| (1,3440) | 1:31:A:LYS:HE2  | 1:32:A:GLU:HG2  | 20       | 0.11          |
| (1,3436) | 1:29:A:SER:HA   | 1:31:A:LYS:HE3  | 9        | 0.11          |
| (1,3432) | 1:28:A:LEU:HD21 | 1:35:A:GLU:H    | 20       | 0.11          |
| (1,3432) | 1:28:A:LEU:HD22 | 1:35:A:GLU:H    | 20       | 0.11          |
| (1,3432) | 1:28:A:LEU:HD23 | 1:35:A:GLU:H    | 20       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 6        | 0.11          |
| (1,3426) | 1:27:A:LYS:HB3  | 1:70:A:ASP:HB3  | 7        | 0.11          |
| (1,3421) | 1:20:A:GLY:HA3  | 1:21:A:LYS:HE2  | 8        | 0.11          |
| (1,3421) | 1:20:A:GLY:HA3  | 1:21:A:LYS:HE2  | 11       | 0.11          |
| (1,3420) | 1:19:A:SER:HB3  | 1:25:A:LYS:HB2  | 10       | 0.11          |
| (1,3415) | 1:16:A:HIS:H    | 1:74:A:TYR:HE2  | 15       | 0.11          |
| (1,3405) | 1:14:A:VAL:HA   | 1:74:A:TYR:HE2  | 12       | 0.11          |
| (1,3394) | 1:6:A:THR:HG21  | 1:9:A:GLU:HA    | 8        | 0.11          |
| (1,3394) | 1:6:A:THR:HG22  | 1:9:A:GLU:HA    | 8        | 0.11          |
| (1,3394) | 1:6:A:THR:HG23  | 1:9:A:GLU:HA    | 8        | 0.11          |
| (1,3392) | 1:66:B:ASP:HB2  | 1:68:B:GLU:H    | 5        | 0.11          |
| (1,3385) | 1:66:A:ASP:HB2  | 1:68:A:GLU:H    | 5        | 0.11          |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 7        | 0.11          |
| (1,3273) | 1:11:B:LEU:HA   | 1:13:B:ASN:HD21 | 11       | 0.11          |
| (1,3271) | 1:11:A:LEU:HA   | 1:13:A:ASN:HD21 | 7        | 0.11          |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD11 | 6        | 0.11          |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD12 | 6        | 0.11          |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD13 | 6        | 0.11          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 1        | 0.11          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 5        | 0.11          |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 8        | 0.11          |
| (1,3201) | 1:45:A:LEU:HD11 | 1:46:A:ASP:HB3  | 1        | 0.11          |
| (1,3201) | 1:45:A:LEU:HD12 | 1:46:A:ASP:HB3  | 1        | 0.11          |
| (1,3201) | 1:45:A:LEU:HD13 | 1:46:A:ASP:HB3  | 1        | 0.11          |
| (1,3201) | 1:45:A:LEU:HD11 | 1:46:A:ASP:HB3  | 20       | 0.11          |
| (1,3201) | 1:45:A:LEU:HD12 | 1:46:A:ASP:HB3  | 20       | 0.11          |
| (1,3201) | 1:45:A:LEU:HD13 | 1:46:A:ASP:HB3  | 20       | 0.11          |
| (1,3194) | 1:33:B:LEU:HG   | 1:69:B:VAL:HA   | 9        | 0.11          |
| (1,3181) | 1:27:B:LYS:HE3  | 1:71:B:PHE:H    | 20       | 0.11          |
| (1,3050) | 1:49:B:LYS:H    | 1:50:B:ASP:HB2  | 11       | 0.11          |
| (1,2917) | 1:19:B:SER:HB2  | 1:28:B:LEU:HB2  | 6        | 0.11          |
| (1,2625) | 1:30:A:LYS:H    | 1:68:A:GLU:HG3  | 4        | 0.11          |
| (1,2563) | 1:31:A:LYS:HG3  | 1:32:A:GLU:HG3  | 20       | 0.11          |
| (1,2454) | 1:30:B:LYS:HG2  | 1:31:B:LYS:HE2  | 2        | 0.11          |
| (1,2364) | 1:90:A:TRP:HA   | 1:91:A:GLU:HG2  | 19       | 0.11          |
| (1,2304) | 1:29:B:SER:HA   | 1:31:B:LYS:HG2  | 6        | 0.11          |
| (1,2234) | 1:30:A:LYS:H    | 1:30:A:LYS:HG2  | 6        | 0.11          |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG21 | 4        | 0.11          |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG22 | 4        | 0.11          |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG23 | 4        | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 7        | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 7        | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 13       | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 13       | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 13       | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG21 | 16       | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG22 | 16       | 0.11          |
| (1,2151) | 1:37:B:LEU:HA   | 1:39:B:THR:HG23 | 16       | 0.11          |
| (1,2128) | 1:64:B:ASN:HB3  | 1:73:B:GLU:HB2  | 16       | 0.11          |
| (1,2124) | 1:64:A:ASN:HB3  | 1:73:A:GLU:HB2  | 7        | 0.11          |
| (1,2103) | 1:63:A:GLU:HB2  | 1:64:A:ASN:HD21 | 7        | 0.11          |
| (1,1930) | 1:63:B:GLU:H    | 1:63:B:GLU:HG3  | 5        | 0.11          |
| (1,1843) | 1:31:B:LYS:HG2  | 1:32:B:GLU:H    | 17       | 0.11          |
| (1,1833) | 1:25:A:LYS:HB2  | 1:26:A:TYR:HE1  | 10       | 0.11          |
| (1,1754) | 1:30:B:LYS:HE3  | 1:69:B:VAL:HA   | 1        | 0.11          |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 10       | 0.11          |
| (1,1677) | 1:24:B:ASP:HB2  | 1:27:B:LYS:HG3  | 7        | 0.11          |
| (1,1650) | 1:74:B:TYR:HE1  | 1:78:B:VAL:HG21 | 18       | 0.11          |
| (1,1650) | 1:74:B:TYR:HE1  | 1:78:B:VAL:HG22 | 18       | 0.11          |
| (1,1650) | 1:74:B:TYR:HE1  | 1:78:B:VAL:HG23 | 18       | 0.11          |
| (1,1623) | 1:30:B:LYS:HE2  | 1:33:B:LEU:HB3  | 5        | 0.11          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG11 | 14       | 0.11          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG12 | 14       | 0.11          |
| (1,1613) | 1:11:A:LEU:HG   | 1:75:A:VAL:HG13 | 14       | 0.11          |
| (1,1608) | 1:27:A:LYS:HD2  | 1:70:A:ASP:HB3  | 1        | 0.11          |
| (1,1606) | 1:83:B:VAL:HG11 | 1:84:B:ALA:H    | 3        | 0.11          |
| (1,1606) | 1:83:B:VAL:HG12 | 1:84:B:ALA:H    | 3        | 0.11          |
| (1,1606) | 1:83:B:VAL:HG13 | 1:84:B:ALA:H    | 3        | 0.11          |
| (1,1600) | 1:83:A:VAL:HG11 | 1:84:A:ALA:H    | 10       | 0.11          |
| (1,1600) | 1:83:A:VAL:HG12 | 1:84:A:ALA:H    | 10       | 0.11          |
| (1,1600) | 1:83:A:VAL:HG13 | 1:84:A:ALA:H    | 10       | 0.11          |
| (1,1593) | 1:25:B:LYS:HB2  | 1:25:B:LYS:HE3  | 14       | 0.11          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 2        | 0.11          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 4        | 0.11          |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 6        | 0.11          |
| (1,1588) | 1:25:A:LYS:HB2  | 1:25:A:LYS:HE3  | 20       | 0.11          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD21  | 1        | 0.11          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD22  | 1        | 0.11          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD23  | 1        | 0.11          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD21  | 9        | 0.11          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD22  | 9        | 0.11          |
| (1,1578) | 1:4:B:LEU:H     | 1:4:B:LEU:HD23  | 9        | 0.11          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 2        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 2        | 0.11          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 2        | 0.11          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD21  | 5        | 0.11          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD22  | 5        | 0.11          |
| (1,1571) | 1:4:A:LEU:H     | 1:4:A:LEU:HD23  | 5        | 0.11          |
| (1,1504) | 1:76:B:VAL:HG21 | 1:80:B:ALA:H    | 13       | 0.11          |
| (1,1504) | 1:76:B:VAL:HG22 | 1:80:B:ALA:H    | 13       | 0.11          |
| (1,1504) | 1:76:B:VAL:HG23 | 1:80:B:ALA:H    | 13       | 0.11          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 4        | 0.11          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 4        | 0.11          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 4        | 0.11          |
| (1,1492) | 1:36:A:LEU:HD11 | 1:74:A:TYR:HD1  | 13       | 0.11          |
| (1,1492) | 1:36:A:LEU:HD12 | 1:74:A:TYR:HD1  | 13       | 0.11          |
| (1,1492) | 1:36:A:LEU:HD13 | 1:74:A:TYR:HD1  | 13       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD21 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD22 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG21 | 1:81:B:LEU:HD23 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD21 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD22 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG22 | 1:81:B:LEU:HD23 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD21 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD22 | 12       | 0.11          |
| (1,1407) | 1:54:B:VAL:HG23 | 1:81:B:LEU:HD23 | 12       | 0.11          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD21 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD22 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG21 | 1:81:A:LEU:HD23 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD21 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD22 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG22 | 1:81:A:LEU:HD23 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD21 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD22 | 3        | 0.11          |
| (1,1402) | 1:54:A:VAL:HG23 | 1:81:A:LEU:HD23 | 3        | 0.11          |
| (1,1395) | 1:31:B:LYS:HB2  | 1:32:B:GLU:H    | 7        | 0.11          |
| (1,1377) | 1:44:B:PHE:HA   | 1:85:B:MET:HE1  | 19       | 0.11          |
| (1,1377) | 1:44:B:PHE:HA   | 1:85:B:MET:HE2  | 19       | 0.11          |
| (1,1377) | 1:44:B:PHE:HA   | 1:85:B:MET:HE3  | 19       | 0.11          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 8        | 0.11          |
| (1,1328) | 1:29:B:SER:HB2  | 1:31:B:LYS:HG3  | 9        | 0.11          |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 6        | 0.11          |
| (1,1275) | 1:21:B:LYS:HB2  | 1:32:B:GLU:HG3  | 14       | 0.11          |
| (1,1269) | 1:41:A:LEU:HD21 | 1:78:A:VAL:HA   | 15       | 0.11          |
| (1,1269) | 1:41:A:LEU:HD22 | 1:78:A:VAL:HA   | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1269) | 1:41:A:LEU:HD23 | 1:78:A:VAL:HA   | 15       | 0.11          |
| (1,1234) | 1:91:B:GLU:H    | 1:91:B:GLU:HG2  | 19       | 0.11          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 10       | 0.11          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 10       | 0.11          |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 10       | 0.11          |
| (1,1221) | 1:41:A:LEU:HB3  | 1:44:A:PHE:HB2  | 14       | 0.11          |
| (1,1202) | 1:88:A:PHE:HD1  | 1:85:A:MET:HE1  | 11       | 0.11          |
| (1,1202) | 1:88:A:PHE:HD1  | 1:85:A:MET:HE2  | 11       | 0.11          |
| (1,1202) | 1:88:A:PHE:HD1  | 1:85:A:MET:HE3  | 11       | 0.11          |
| (1,1202) | 1:88:A:PHE:HD2  | 1:85:A:MET:HE1  | 11       | 0.11          |
| (1,1202) | 1:88:A:PHE:HD2  | 1:85:A:MET:HE2  | 11       | 0.11          |
| (1,1202) | 1:88:A:PHE:HD2  | 1:85:A:MET:HE3  | 11       | 0.11          |
| (1,1201) | 1:88:A:PHE:HD1  | 1:85:A:MET:HE1  | 11       | 0.11          |
| (1,1201) | 1:88:A:PHE:HD1  | 1:85:A:MET:HE2  | 11       | 0.11          |
| (1,1201) | 1:88:A:PHE:HD1  | 1:85:A:MET:HE3  | 11       | 0.11          |
| (1,1201) | 1:88:A:PHE:HD2  | 1:85:A:MET:HE1  | 11       | 0.11          |
| (1,1201) | 1:88:A:PHE:HD2  | 1:85:A:MET:HE2  | 11       | 0.11          |
| (1,1201) | 1:88:A:PHE:HD2  | 1:85:A:MET:HE3  | 11       | 0.11          |
| (1,1005) | 1:15:B:PHE:HE2  | 1:27:B:LYS:HA   | 17       | 0.11          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG11 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG12 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD21 | 1:78:B:VAL:HG13 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG11 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG12 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD22 | 1:78:B:VAL:HG13 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG11 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG12 | 8        | 0.11          |
| (1,995)  | 1:37:B:LEU:HD23 | 1:78:B:VAL:HG13 | 8        | 0.11          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 17       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG11 | 18       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG12 | 18       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD21 | 1:78:A:VAL:HG13 | 18       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG11 | 18       | 0.11          |
| (1,988)  | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG12 | 18       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,988) | 1:37:A:LEU:HD22 | 1:78:A:VAL:HG13 | 18       | 0.11          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG11 | 18       | 0.11          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG12 | 18       | 0.11          |
| (1,988) | 1:37:A:LEU:HD23 | 1:78:A:VAL:HG13 | 18       | 0.11          |
| (1,987) | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG11 | 10       | 0.11          |
| (1,987) | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG12 | 10       | 0.11          |
| (1,987) | 1:30:A:LYS:HD2  | 1:69:A:VAL:HG13 | 10       | 0.11          |
| (1,967) | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 4        | 0.11          |
| (1,967) | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 4        | 0.11          |
| (1,967) | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 4        | 0.11          |
| (1,963) | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 1        | 0.11          |
| (1,963) | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 7        | 0.11          |
| (1,963) | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 11       | 0.11          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 2        | 0.11          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 2        | 0.11          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 2        | 0.11          |
| (1,956) | 1:54:A:VAL:HG11 | 1:55:A:ASP:H    | 11       | 0.11          |
| (1,956) | 1:54:A:VAL:HG12 | 1:55:A:ASP:H    | 11       | 0.11          |
| (1,956) | 1:54:A:VAL:HG13 | 1:55:A:ASP:H    | 11       | 0.11          |
| (1,951) | 1:27:A:LYS:HA   | 1:27:A:LYS:HD2  | 9        | 0.11          |
| (1,892) | 1:44:B:PHE:HE2  | 1:82:B:THR:HA   | 17       | 0.11          |
| (1,859) | 1:75:A:VAL:H    | 1:75:A:VAL:HG21 | 15       | 0.11          |
| (1,859) | 1:75:A:VAL:H    | 1:75:A:VAL:HG22 | 15       | 0.11          |
| (1,859) | 1:75:A:VAL:H    | 1:75:A:VAL:HG23 | 15       | 0.11          |
| (1,858) | 1:31:A:LYS:HB3  | 1:31:A:LYS:HE2  | 4        | 0.11          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD11 | 14       | 0.11          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD12 | 14       | 0.11          |
| (1,731) | 1:18:B:HIS:HB3  | 1:28:B:LEU:HD13 | 14       | 0.11          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD11 | 19       | 0.11          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD12 | 19       | 0.11          |
| (1,726) | 1:18:A:HIS:HB3  | 1:28:A:LEU:HD13 | 19       | 0.11          |
| (1,695) | 1:4:A:LEU:HB2   | 1:4:A:LEU:HD21  | 17       | 0.11          |
| (1,695) | 1:4:A:LEU:HB2   | 1:4:A:LEU:HD22  | 17       | 0.11          |
| (1,695) | 1:4:A:LEU:HB2   | 1:4:A:LEU:HD23  | 17       | 0.11          |
| (1,674) | 1:38:A:GLN:H    | 1:38:A:GLN:HG2  | 15       | 0.11          |
| (1,667) | 1:24:B:ASP:HB3  | 1:27:B:LYS:HB2  | 10       | 0.11          |
| (1,665) | 1:39:A:THR:HG21 | 1:40:A:GLU:HG2  | 1        | 0.11          |
| (1,665) | 1:39:A:THR:HG22 | 1:40:A:GLU:HG2  | 1        | 0.11          |
| (1,665) | 1:39:A:THR:HG23 | 1:40:A:GLU:HG2  | 1        | 0.11          |
| (1,621) | 1:9:A:GLU:HA    | 1:12:A:ILE:HB   | 4        | 0.11          |
| (1,613) | 1:25:B:LYS:HG3  | 1:25:B:LYS:HE3  | 1        | 0.11          |
| (1,600) | 1:83:B:VAL:H    | 1:83:B:VAL:HG11 | 9        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,600) | 1:83:B:VAL:H    | 1:83:B:VAL:HG12 | 9        | 0.11          |
| (1,600) | 1:83:B:VAL:H    | 1:83:B:VAL:HG13 | 9        | 0.11          |
| (1,575) | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 2        | 0.11          |
| (1,575) | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 2        | 0.11          |
| (1,575) | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 2        | 0.11          |
| (1,575) | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 3        | 0.11          |
| (1,575) | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 3        | 0.11          |
| (1,575) | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 3        | 0.11          |
| (1,575) | 1:28:B:LEU:HD11 | 1:32:B:GLU:HB2  | 14       | 0.11          |
| (1,575) | 1:28:B:LEU:HD12 | 1:32:B:GLU:HB2  | 14       | 0.11          |
| (1,575) | 1:28:B:LEU:HD13 | 1:32:B:GLU:HB2  | 14       | 0.11          |
| (1,564) | 1:14:B:VAL:H    | 1:14:B:VAL:HB   | 9        | 0.11          |
| (1,557) | 1:14:A:VAL:H    | 1:14:A:VAL:HB   | 3        | 0.11          |
| (1,549) | 1:3:B:GLU:HA    | 1:3:B:GLU:HG2   | 9        | 0.11          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 3        | 0.11          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 3        | 0.11          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 3        | 0.11          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG11 | 15       | 0.11          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG12 | 15       | 0.11          |
| (1,535) | 1:80:A:ALA:HA   | 1:83:A:VAL:HG13 | 15       | 0.11          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 1        | 0.11          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 1        | 0.11          |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 1        | 0.11          |
| (1,505) | 1:57:B:VAL:HG21 | 1:81:B:LEU:HG   | 10       | 0.11          |
| (1,505) | 1:57:B:VAL:HG22 | 1:81:B:LEU:HG   | 10       | 0.11          |
| (1,505) | 1:57:B:VAL:HG23 | 1:81:B:LEU:HG   | 10       | 0.11          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD11  | 5        | 0.11          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD12  | 5        | 0.11          |
| (1,447) | 1:4:B:LEU:HA    | 1:4:B:LEU:HD13  | 5        | 0.11          |
| (1,440) | 1:60:B:GLU:H    | 1:60:B:GLU:HB2  | 6        | 0.11          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 8        | 0.11          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 8        | 0.11          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 8        | 0.11          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 19       | 0.11          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 19       | 0.11          |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 19       | 0.11          |
| (1,435) | 1:26:B:TYR:HB2  | 1:26:B:TYR:HD2  | 11       | 0.11          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 1        | 0.11          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 1        | 0.11          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 1        | 0.11          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 20       | 0.11          |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 20       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 20       | 0.11          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG21 | 2        | 0.11          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG22 | 2        | 0.11          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG23 | 2        | 0.11          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG21 | 10       | 0.11          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG22 | 10       | 0.11          |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG23 | 10       | 0.11          |
| (1,353) | 1:37:B:LEU:HB3  | 1:77:B:LEU:HD21 | 15       | 0.11          |
| (1,353) | 1:37:B:LEU:HB3  | 1:77:B:LEU:HD22 | 15       | 0.11          |
| (1,353) | 1:37:B:LEU:HB3  | 1:77:B:LEU:HD23 | 15       | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 8        | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 9        | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 11       | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 13       | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 13       | 0.11          |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 13       | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 13       | 0.11          |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 13       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 13       | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 13       | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 13       | 0.11          |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 13       | 0.11          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 1        | 0.11          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 10       | 0.11          |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 10       | 0.11          |
| (1,311) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HD2  | 16       | 0.11          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD11 | 6        | 0.11          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD12 | 6        | 0.11          |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD13 | 6        | 0.11          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 9        | 0.11          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 9        | 0.11          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 9        | 0.11          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 11       | 0.11          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 11       | 0.11          |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 11       | 0.11          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 11       | 0.11          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 11       | 0.11          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 11       | 0.11          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD21 | 17       | 0.11          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD22 | 17       | 0.11          |
| (1,286) | 1:37:A:LEU:HA   | 1:37:A:LEU:HD23 | 17       | 0.11          |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB1  | 19       | 0.11          |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB2  | 19       | 0.11          |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB3  | 19       | 0.11          |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB1  | 19       | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB2 | 19       | 0.11          |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB3 | 19       | 0.11          |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB1 | 19       | 0.11          |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB2 | 19       | 0.11          |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB3 | 19       | 0.11          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3 | 3        | 0.11          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB1 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB2 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG11 | 1:80:A:ALA:HB3 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB1 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB2 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG12 | 1:80:A:ALA:HB3 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB1 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB2 | 12       | 0.11          |
| (1,274) | 1:57:A:VAL:HG13 | 1:80:A:ALA:HB3 | 12       | 0.11          |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2 | 15       | 0.11          |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2 | 15       | 0.11          |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2 | 15       | 0.11          |
| (1,259) | 1:37:A:LEU:HD21 | 1:41:A:LEU:HB2 | 3        | 0.11          |
| (1,259) | 1:37:A:LEU:HD22 | 1:41:A:LEU:HB2 | 3        | 0.11          |
| (1,259) | 1:37:A:LEU:HD23 | 1:41:A:LEU:HB2 | 3        | 0.11          |
| (1,259) | 1:37:A:LEU:HD21 | 1:41:A:LEU:HB2 | 4        | 0.11          |
| (1,259) | 1:37:A:LEU:HD22 | 1:41:A:LEU:HB2 | 4        | 0.11          |
| (1,259) | 1:37:A:LEU:HD23 | 1:41:A:LEU:HB2 | 4        | 0.11          |
| (1,259) | 1:37:A:LEU:HD21 | 1:41:A:LEU:HB2 | 15       | 0.11          |
| (1,259) | 1:37:A:LEU:HD22 | 1:41:A:LEU:HB2 | 15       | 0.11          |
| (1,259) | 1:37:A:LEU:HD23 | 1:41:A:LEU:HB2 | 15       | 0.11          |
| (1,241) | 1:86:A:ASN:HB3  | 1:12:B:ILE:HB  | 7        | 0.11          |
| (1,207) | 1:91:A:GLU:HB2  | 1:26:B:TYR:HE1 | 20       | 0.11          |
| (1,203) | 1:90:A:TRP:HB2  | 1:26:B:TYR:HE1 | 12       | 0.11          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2 | 6        | 0.11          |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2 | 20       | 0.11          |
| (1,168) | 1:83:A:VAL:HG11 | 1:72:B:GLN:HG3 | 3        | 0.11          |
| (1,168) | 1:83:A:VAL:HG12 | 1:72:B:GLN:HG3 | 3        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,168) | 1:83:A:VAL:HG13 | 1:72:B:GLN:HG3  | 3        | 0.11          |
| (1,166) | 1:83:A:VAL:HG11 | 1:72:B:GLN:HB2  | 2        | 0.11          |
| (1,166) | 1:83:A:VAL:HG12 | 1:72:B:GLN:HB2  | 2        | 0.11          |
| (1,166) | 1:83:A:VAL:HG13 | 1:72:B:GLN:HB2  | 2        | 0.11          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 1        | 0.11          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 1        | 0.11          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 1        | 0.11          |
| (1,165) | 1:83:A:VAL:HG21 | 1:72:B:GLN:HB2  | 18       | 0.11          |
| (1,165) | 1:83:A:VAL:HG22 | 1:72:B:GLN:HB2  | 18       | 0.11          |
| (1,165) | 1:83:A:VAL:HG23 | 1:72:B:GLN:HB2  | 18       | 0.11          |
| (1,155) | 1:14:A:VAL:HG21 | 1:4:B:LEU:H     | 3        | 0.11          |
| (1,155) | 1:14:A:VAL:HG22 | 1:4:B:LEU:H     | 3        | 0.11          |
| (1,155) | 1:14:A:VAL:HG23 | 1:4:B:LEU:H     | 3        | 0.11          |
| (1,144) | 1:11:A:LEU:HD11 | 1:4:B:LEU:HB2   | 8        | 0.11          |
| (1,144) | 1:11:A:LEU:HD12 | 1:4:B:LEU:HB2   | 8        | 0.11          |
| (1,144) | 1:11:A:LEU:HD13 | 1:4:B:LEU:HB2   | 8        | 0.11          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 5        | 0.11          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG21 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG22 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB1  | 1:75:B:VAL:HG23 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG21 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG22 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB2  | 1:75:B:VAL:HG23 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG21 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG22 | 16       | 0.11          |
| (1,137) | 1:79:A:ALA:HB3  | 1:75:B:VAL:HG23 | 16       | 0.11          |
| (1,94)  | 1:75:A:VAL:HG11 | 1:80:B:ALA:HA   | 19       | 0.11          |
| (1,94)  | 1:75:A:VAL:HG12 | 1:80:B:ALA:HA   | 19       | 0.11          |
| (1,94)  | 1:75:A:VAL:HG13 | 1:80:B:ALA:HA   | 19       | 0.11          |
| (1,85)  | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 1        | 0.11          |
| (1,85)  | 1:3:A:GLU:HG2   | 1:10:B:THR:HB   | 17       | 0.11          |
| (1,81)  | 1:72:A:GLN:HA   | 1:80:B:ALA:HA   | 14       | 0.11          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG21 | 4        | 0.11          |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG22 | 4        | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,75)   | 1:4:A:LEU:HD21 | 1:14:B:VAL:HG23 | 4        | 0.11          |
| (1,75)   | 1:4:A:LEU:HD22 | 1:14:B:VAL:HG21 | 4        | 0.11          |
| (1,75)   | 1:4:A:LEU:HD22 | 1:14:B:VAL:HG22 | 4        | 0.11          |
| (1,75)   | 1:4:A:LEU:HD22 | 1:14:B:VAL:HG23 | 4        | 0.11          |
| (1,75)   | 1:4:A:LEU:HD23 | 1:14:B:VAL:HG21 | 4        | 0.11          |
| (1,75)   | 1:4:A:LEU:HD23 | 1:14:B:VAL:HG22 | 4        | 0.11          |
| (1,75)   | 1:4:A:LEU:HD23 | 1:14:B:VAL:HG23 | 4        | 0.11          |
| (1,75)   | 1:4:A:LEU:HD21 | 1:14:B:VAL:HG21 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD21 | 1:14:B:VAL:HG22 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD21 | 1:14:B:VAL:HG23 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD22 | 1:14:B:VAL:HG21 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD22 | 1:14:B:VAL:HG22 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD22 | 1:14:B:VAL:HG23 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD23 | 1:14:B:VAL:HG21 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD23 | 1:14:B:VAL:HG22 | 11       | 0.11          |
| (1,75)   | 1:4:A:LEU:HD23 | 1:14:B:VAL:HG23 | 11       | 0.11          |
| (1,74)   | 1:4:A:LEU:HB3  | 1:14:B:VAL:HG21 | 14       | 0.11          |
| (1,74)   | 1:4:A:LEU:HB3  | 1:14:B:VAL:HG22 | 14       | 0.11          |
| (1,74)   | 1:4:A:LEU:HB3  | 1:14:B:VAL:HG23 | 14       | 0.11          |
| (1,56)   | 1:71:A:PHE:HD2 | 1:83:B:VAL:HB   | 7        | 0.11          |
| (1,40)   | 1:4:A:LEU:HD21 | 1:40:B:GLU:HG3  | 17       | 0.11          |
| (1,40)   | 1:4:A:LEU:HD22 | 1:40:B:GLU:HG3  | 17       | 0.11          |
| (1,40)   | 1:4:A:LEU:HD23 | 1:40:B:GLU:HG3  | 17       | 0.11          |
| (1,39)   | 1:4:A:LEU:HD21 | 1:40:B:GLU:HA   | 1        | 0.11          |
| (1,39)   | 1:4:A:LEU:HD22 | 1:40:B:GLU:HA   | 1        | 0.11          |
| (1,39)   | 1:4:A:LEU:HD23 | 1:40:B:GLU:HA   | 1        | 0.11          |
| (1,39)   | 1:4:A:LEU:HD21 | 1:40:B:GLU:HA   | 16       | 0.11          |
| (1,39)   | 1:4:A:LEU:HD22 | 1:40:B:GLU:HA   | 16       | 0.11          |
| (1,39)   | 1:4:A:LEU:HD23 | 1:40:B:GLU:HA   | 16       | 0.11          |
| (1,3647) | 1:91:B:GLU:HB2 | 1:93:B:SER:H    | 4        | 0.1           |
| (1,3642) | 1:86:B:ASN:HB2 | 1:87:B:ASN:HB2  | 17       | 0.1           |
| (1,3618) | 1:63:B:GLU:HG3 | 1:64:B:ASN:HB2  | 9        | 0.1           |
| (1,3618) | 1:63:B:GLU:HG3 | 1:64:B:ASN:HB2  | 10       | 0.1           |
| (1,3617) | 1:63:B:GLU:HA  | 1:66:B:ASP:HB2  | 10       | 0.1           |
| (1,3605) | 1:51:B:VAL:HB  | 1:52:B:ASP:HB3  | 11       | 0.1           |
| (1,3575) | 1:37:B:LEU:HB2 | 1:74:B:TYR:HA   | 16       | 0.1           |
| (1,3572) | 1:34:B:LYS:HA  | 1:36:B:LEU:HD21 | 4        | 0.1           |
| (1,3572) | 1:34:B:LYS:HA  | 1:36:B:LEU:HD22 | 4        | 0.1           |
| (1,3572) | 1:34:B:LYS:HA  | 1:36:B:LEU:HD23 | 4        | 0.1           |
| (1,3571) | 1:33:B:LEU:HB3 | 1:36:B:LEU:HG   | 5        | 0.1           |
| (1,3568) | 1:31:B:LYS:HE2 | 1:32:B:GLU:HG2  | 20       | 0.1           |
| (1,3556) | 1:27:B:LYS:HE3 | 1:69:B:VAL:H    | 1        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3552) | 1:25:B:LYS:HG2  | 1:26:B:TYR:HE1  | 5        | 0.1           |
| (1,3549) | 1:20:B:GLY:HA3  | 1:21:B:LYS:HE2  | 19       | 0.1           |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 8        | 0.1           |
| (1,3548) | 1:19:B:SER:HB3  | 1:25:B:LYS:HB2  | 17       | 0.1           |
| (1,3528) | 1:9:B:GLU:HA    | 1:71:B:PHE:HE2  | 17       | 0.1           |
| (1,3492) | 1:68:A:GLU:HB3  | 1:70:A:ASP:HB3  | 11       | 0.1           |
| (1,3487) | 1:58:A:MET:HG2  | 1:59:A:LYS:HB2  | 2        | 0.1           |
| (1,3485) | 1:58:A:MET:HA   | 1:77:A:LEU:HG   | 2        | 0.1           |
| (1,3470) | 1:48:A:GLN:HE22 | 1:49:A:LYS:H    | 18       | 0.1           |
| (1,3469) | 1:48:A:GLN:HE21 | 1:50:A:ASP:H    | 10       | 0.1           |
| (1,3413) | 1:15:A:PHE:HD2  | 1:19:A:SER:HA   | 1        | 0.1           |
| (1,3405) | 1:14:A:VAL:HA   | 1:74:A:TYR:HE2  | 3        | 0.1           |
| (1,3400) | 1:9:A:GLU:HA    | 1:71:A:PHE:HE2  | 10       | 0.1           |
| (1,3400) | 1:9:A:GLU:HA    | 1:71:A:PHE:HE2  | 15       | 0.1           |
| (1,3279) | 1:26:B:TYR:HA   | 1:27:B:LYS:HD2  | 11       | 0.1           |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD11 | 15       | 0.1           |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD12 | 15       | 0.1           |
| (1,3267) | 1:14:B:VAL:H    | 1:36:B:LEU:HD13 | 15       | 0.1           |
| (1,3236) | 1:59:A:LYS:H    | 1:60:A:GLU:HB3  | 3        | 0.1           |
| (1,2912) | 1:41:A:LEU:HA   | 1:45:A:LEU:HD21 | 9        | 0.1           |
| (1,2912) | 1:41:A:LEU:HA   | 1:45:A:LEU:HD22 | 9        | 0.1           |
| (1,2912) | 1:41:A:LEU:HA   | 1:45:A:LEU:HD23 | 9        | 0.1           |
| (1,2844) | 1:91:B:GLU:HB2  | 1:93:B:SER:HB2  | 20       | 0.1           |
| (1,2782) | 1:25:A:LYS:HG3  | 1:26:A:TYR:HE1  | 3        | 0.1           |
| (1,2549) | 1:16:B:HIS:HE1  | 1:26:B:TYR:HB3  | 19       | 0.1           |
| (1,2538) | 1:30:B:LYS:HD2  | 1:69:B:VAL:HA   | 12       | 0.1           |
| (1,2515) | 1:19:A:SER:HB2  | 1:25:A:LYS:HA   | 4        | 0.1           |
| (1,2476) | 1:59:B:LYS:HG3  | 1:60:B:GLU:HB2  | 19       | 0.1           |
| (1,2448) | 1:30:A:LYS:HG2  | 1:31:A:LYS:HE2  | 20       | 0.1           |
| (1,2370) | 1:90:B:TRP:HA   | 1:91:B:GLU:HG2  | 4        | 0.1           |
| (1,2239) | 1:30:B:LYS:H    | 1:30:B:LYS:HG2  | 3        | 0.1           |
| (1,2234) | 1:30:A:LYS:H    | 1:30:A:LYS:HG2  | 16       | 0.1           |
| (1,2217) | 1:37:B:LEU:H    | 1:39:B:THR:HG21 | 8        | 0.1           |
| (1,2217) | 1:37:B:LEU:H    | 1:39:B:THR:HG22 | 8        | 0.1           |
| (1,2217) | 1:37:B:LEU:H    | 1:39:B:THR:HG23 | 8        | 0.1           |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG21 | 1        | 0.1           |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG22 | 1        | 0.1           |
| (1,2212) | 1:37:A:LEU:H    | 1:39:A:THR:HG23 | 1        | 0.1           |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD21  | 4        | 0.1           |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD22  | 4        | 0.1           |
| (1,1927) | 1:2:B:SER:HA    | 1:4:B:LEU:HD23  | 4        | 0.1           |
| (1,1684) | 1:55:B:ASP:HB3  | 1:56:B:LYS:HD2  | 9        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1669) | 1:30:A:LYS:HA   | 1:33:A:LEU:HB3  | 16       | 0.1           |
| (1,1664) | 1:54:B:VAL:HA   | 1:81:B:LEU:HG   | 14       | 0.1           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 7        | 0.1           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 7        | 0.1           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 7        | 0.1           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG11 | 12       | 0.1           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG12 | 12       | 0.1           |
| (1,1620) | 1:11:B:LEU:HG   | 1:75:B:VAL:HG13 | 12       | 0.1           |
| (1,1589) | 1:41:A:LEU:HB2  | 1:45:A:LEU:HB3  | 9        | 0.1           |
| (1,1530) | 1:24:A:ASP:HB2  | 1:27:A:LYS:HG2  | 20       | 0.1           |
| (1,1323) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG3  | 4        | 0.1           |
| (1,1294) | 1:37:B:LEU:HD21 | 1:74:B:TYR:HE1  | 10       | 0.1           |
| (1,1294) | 1:37:B:LEU:HD22 | 1:74:B:TYR:HE1  | 10       | 0.1           |
| (1,1294) | 1:37:B:LEU:HD23 | 1:74:B:TYR:HE1  | 10       | 0.1           |
| (1,1269) | 1:41:A:LEU:HD21 | 1:78:A:VAL:HA   | 19       | 0.1           |
| (1,1269) | 1:41:A:LEU:HD22 | 1:78:A:VAL:HA   | 19       | 0.1           |
| (1,1269) | 1:41:A:LEU:HD23 | 1:78:A:VAL:HA   | 19       | 0.1           |
| (1,1267) | 1:21:A:LYS:HB2  | 1:32:A:GLU:HG3  | 7        | 0.1           |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG21 | 6        | 0.1           |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG22 | 6        | 0.1           |
| (1,1232) | 1:75:B:VAL:HA   | 1:78:B:VAL:HG23 | 6        | 0.1           |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 4        | 0.1           |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 4        | 0.1           |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 4        | 0.1           |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG21 | 7        | 0.1           |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG22 | 7        | 0.1           |
| (1,1223) | 1:75:A:VAL:HA   | 1:78:A:VAL:HG23 | 7        | 0.1           |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE1  | 2        | 0.1           |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE2  | 2        | 0.1           |
| (1,1106) | 1:44:B:PHE:HD2  | 1:85:B:MET:HE3  | 2        | 0.1           |
| (1,1066) | 1:78:A:VAL:H    | 1:78:A:VAL:HG21 | 2        | 0.1           |
| (1,1066) | 1:78:A:VAL:H    | 1:78:A:VAL:HG22 | 2        | 0.1           |
| (1,1066) | 1:78:A:VAL:H    | 1:78:A:VAL:HG23 | 2        | 0.1           |
| (1,1049) | 1:75:B:VAL:HG21 | 1:76:B:VAL:H    | 9        | 0.1           |
| (1,1049) | 1:75:B:VAL:HG22 | 1:76:B:VAL:H    | 9        | 0.1           |
| (1,1049) | 1:75:B:VAL:HG23 | 1:76:B:VAL:H    | 9        | 0.1           |
| (1,1041) | 1:75:A:VAL:HG21 | 1:76:A:VAL:H    | 16       | 0.1           |
| (1,1041) | 1:75:A:VAL:HG22 | 1:76:A:VAL:H    | 16       | 0.1           |
| (1,1041) | 1:75:A:VAL:HG23 | 1:76:A:VAL:H    | 16       | 0.1           |
| (1,967)  | 1:54:B:VAL:HG11 | 1:55:B:ASP:H    | 9        | 0.1           |
| (1,967)  | 1:54:B:VAL:HG12 | 1:55:B:ASP:H    | 9        | 0.1           |
| (1,967)  | 1:54:B:VAL:HG13 | 1:55:B:ASP:H    | 9        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,963) | 1:29:B:SER:HB3  | 1:68:B:GLU:HG3  | 8        | 0.1           |
| (1,951) | 1:27:A:LYS:HA   | 1:27:A:LYS:HD2  | 10       | 0.1           |
| (1,927) | 1:21:B:LYS:HA   | 1:21:B:LYS:HE2  | 10       | 0.1           |
| (1,859) | 1:75:A:VAL:H    | 1:75:A:VAL:HG21 | 5        | 0.1           |
| (1,859) | 1:75:A:VAL:H    | 1:75:A:VAL:HG22 | 5        | 0.1           |
| (1,859) | 1:75:A:VAL:H    | 1:75:A:VAL:HG23 | 5        | 0.1           |
| (1,767) | 1:58:A:MET:HA   | 1:77:A:LEU:HD11 | 15       | 0.1           |
| (1,767) | 1:58:A:MET:HA   | 1:77:A:LEU:HD12 | 15       | 0.1           |
| (1,767) | 1:58:A:MET:HA   | 1:77:A:LEU:HD13 | 15       | 0.1           |
| (1,760) | 1:46:B:ASP:HA   | 1:49:B:LYS:HG3  | 8        | 0.1           |
| (1,751) | 1:51:B:VAL:HG11 | 1:53:B:ALA:H    | 15       | 0.1           |
| (1,751) | 1:51:B:VAL:HG12 | 1:53:B:ALA:H    | 15       | 0.1           |
| (1,751) | 1:51:B:VAL:HG13 | 1:53:B:ALA:H    | 15       | 0.1           |
| (1,743) | 1:18:B:HIS:HB2  | 1:28:B:LEU:HD11 | 9        | 0.1           |
| (1,743) | 1:18:B:HIS:HB2  | 1:28:B:LEU:HD12 | 9        | 0.1           |
| (1,743) | 1:18:B:HIS:HB2  | 1:28:B:LEU:HD13 | 9        | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD11 | 11       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD12 | 11       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD13 | 11       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD11 | 13       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD12 | 13       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD13 | 13       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD11 | 16       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD12 | 16       | 0.1           |
| (1,739) | 1:12:A:ILE:HA   | 1:12:A:ILE:HD13 | 16       | 0.1           |
| (1,684) | 1:38:B:GLN:H    | 1:38:B:GLN:HG2  | 15       | 0.1           |
| (1,659) | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG21 | 6        | 0.1           |
| (1,659) | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG22 | 6        | 0.1           |
| (1,659) | 1:30:B:LYS:HE3  | 1:69:B:VAL:HG23 | 6        | 0.1           |
| (1,585) | 1:54:A:VAL:H    | 1:54:A:VAL:HG11 | 3        | 0.1           |
| (1,585) | 1:54:A:VAL:H    | 1:54:A:VAL:HG12 | 3        | 0.1           |
| (1,585) | 1:54:A:VAL:H    | 1:54:A:VAL:HG13 | 3        | 0.1           |
| (1,572) | 1:28:A:LEU:HD11 | 1:32:A:GLU:HB2  | 1        | 0.1           |
| (1,572) | 1:28:A:LEU:HD12 | 1:32:A:GLU:HB2  | 1        | 0.1           |
| (1,572) | 1:28:A:LEU:HD13 | 1:32:A:GLU:HB2  | 1        | 0.1           |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG21 | 7        | 0.1           |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG22 | 7        | 0.1           |
| (1,566) | 1:36:B:LEU:HA   | 1:39:B:THR:HG23 | 7        | 0.1           |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG11 | 2        | 0.1           |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG12 | 2        | 0.1           |
| (1,539) | 1:80:B:ALA:HA   | 1:83:B:VAL:HG13 | 2        | 0.1           |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE1  | 9        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE2  | 9        | 0.1           |
| (1,534) | 1:55:A:ASP:HA   | 1:58:A:MET:HE3  | 9        | 0.1           |
| (1,533) | 1:48:A:GLN:HA   | 1:51:A:VAL:HG21 | 10       | 0.1           |
| (1,533) | 1:48:A:GLN:HA   | 1:51:A:VAL:HG22 | 10       | 0.1           |
| (1,533) | 1:48:A:GLN:HA   | 1:51:A:VAL:HG23 | 10       | 0.1           |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG11 | 20       | 0.1           |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG12 | 20       | 0.1           |
| (1,437) | 1:37:B:LEU:HG   | 1:78:B:VAL:HG13 | 20       | 0.1           |
| (1,435) | 1:26:B:TYR:HB2  | 1:26:B:TYR:HD2  | 1        | 0.1           |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG11 | 16       | 0.1           |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG12 | 16       | 0.1           |
| (1,431) | 1:37:A:LEU:HG   | 1:78:A:VAL:HG13 | 16       | 0.1           |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG21 | 17       | 0.1           |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG22 | 17       | 0.1           |
| (1,412) | 1:72:B:GLN:HA   | 1:75:B:VAL:HG23 | 17       | 0.1           |
| (1,406) | 1:72:A:GLN:HA   | 1:75:A:VAL:HG21 | 16       | 0.1           |
| (1,406) | 1:72:A:GLN:HA   | 1:75:A:VAL:HG22 | 16       | 0.1           |
| (1,406) | 1:72:A:GLN:HA   | 1:75:A:VAL:HG23 | 16       | 0.1           |
| (1,395) | 1:29:A:SER:HB2  | 1:31:A:LYS:HG2  | 13       | 0.1           |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD11 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD12 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG21 | 1:12:B:ILE:HD13 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD11 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD12 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG22 | 1:12:B:ILE:HD13 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD11 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD12 | 10       | 0.1           |
| (1,334) | 1:12:B:ILE:HG23 | 1:12:B:ILE:HD13 | 10       | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 3        | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 15       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 15       | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD11 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD12 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG21 | 1:12:A:ILE:HD13 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD11 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD12 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG22 | 1:12:A:ILE:HD13 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD11 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD12 | 20       | 0.1           |
| (1,329) | 1:12:A:ILE:HG23 | 1:12:A:ILE:HD13 | 20       | 0.1           |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD21 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD22 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD21 | 1:36:B:LEU:HD23 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD21 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD22 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD22 | 1:36:B:LEU:HD23 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD21 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD22 | 4        | 0.1           |
| (1,328) | 1:28:B:LEU:HD23 | 1:36:B:LEU:HD23 | 4        | 0.1           |
| (1,314) | 1:56:B:LYS:HB2  | 1:56:B:LYS:HD2  | 12       | 0.1           |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD21 | 4        | 0.1           |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD22 | 4        | 0.1           |
| (1,299) | 1:11:A:LEU:HA   | 1:11:A:LEU:HD23 | 4        | 0.1           |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD11 | 9        | 0.1           |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD12 | 9        | 0.1           |
| (1,298) | 1:77:B:LEU:HA   | 1:77:B:LEU:HD13 | 9        | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 6        | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 6        | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 6        | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 12       | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 12       | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 12       | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD21 | 19       | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD22 | 19       | 0.1           |
| (1,289) | 1:37:B:LEU:HA   | 1:37:B:LEU:HD23 | 19       | 0.1           |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB1  | 16       | 0.1           |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB2  | 16       | 0.1           |
| (1,280) | 1:57:B:VAL:HG21 | 1:80:B:ALA:HB3  | 16       | 0.1           |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB1  | 16       | 0.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB2 | 16       | 0.1           |
| (1,280) | 1:57:B:VAL:HG22 | 1:80:B:ALA:HB3 | 16       | 0.1           |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB1 | 16       | 0.1           |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB2 | 16       | 0.1           |
| (1,280) | 1:57:B:VAL:HG23 | 1:80:B:ALA:HB3 | 16       | 0.1           |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB1 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB2 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG21 | 1:80:A:ALA:HB3 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB1 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB2 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG22 | 1:80:A:ALA:HB3 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB1 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB2 | 18       | 0.1           |
| (1,279) | 1:57:A:VAL:HG23 | 1:80:A:ALA:HB3 | 18       | 0.1           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3 | 4        | 0.1           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB1 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB2 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG11 | 1:80:B:ALA:HB3 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB1 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB2 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG12 | 1:80:B:ALA:HB3 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB1 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB2 | 11       | 0.1           |
| (1,276) | 1:57:B:VAL:HG13 | 1:80:B:ALA:HB3 | 11       | 0.1           |
| (1,267) | 1:37:B:LEU:HD21 | 1:41:B:LEU:HB2 | 20       | 0.1           |
| (1,267) | 1:37:B:LEU:HD22 | 1:41:B:LEU:HB2 | 20       | 0.1           |
| (1,267) | 1:37:B:LEU:HD23 | 1:41:B:LEU:HB2 | 20       | 0.1           |
| (1,241) | 1:86:A:ASN:HB3  | 1:12:B:ILE:HB  | 12       | 0.1           |
| (1,176) | 1:83:A:VAL:HB   | 1:71:B:PHE:HD2 | 11       | 0.1           |
| (1,161) | 1:82:A:THR:HG21 | 1:71:B:PHE:HB2 | 6        | 0.1           |
| (1,161) | 1:82:A:THR:HG22 | 1:71:B:PHE:HB2 | 6        | 0.1           |
| (1,161) | 1:82:A:THR:HG23 | 1:71:B:PHE:HB2 | 6        | 0.1           |
| (1,143) | 1:10:A:THR:HG21 | 1:3:B:GLU:HG3  | 9        | 0.1           |
| (1,143) | 1:10:A:THR:HG22 | 1:3:B:GLU:HG3  | 9        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,143) | 1:10:A:THR:HG23 | 1:3:B:GLU:HG3   | 9        | 0.1           |
| (1,129) | 1:11:A:LEU:HD21 | 1:7:B:ALA:H     | 2        | 0.1           |
| (1,129) | 1:11:A:LEU:HD22 | 1:7:B:ALA:H     | 2        | 0.1           |
| (1,129) | 1:11:A:LEU:HD23 | 1:7:B:ALA:H     | 2        | 0.1           |
| (1,106) | 1:7:A:ALA:H     | 1:10:B:THR:HG21 | 5        | 0.1           |
| (1,106) | 1:7:A:ALA:H     | 1:10:B:THR:HG22 | 5        | 0.1           |
| (1,106) | 1:7:A:ALA:H     | 1:10:B:THR:HG23 | 5        | 0.1           |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB1  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB2  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG21 | 1:79:B:ALA:HB3  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB1  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB2  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG22 | 1:79:B:ALA:HB3  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB1  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB2  | 1        | 0.1           |
| (1,104) | 1:75:A:VAL:HG23 | 1:79:B:ALA:HB3  | 1        | 0.1           |
| (1,94)  | 1:75:A:VAL:HG11 | 1:80:B:ALA:HA   | 9        | 0.1           |
| (1,94)  | 1:75:A:VAL:HG12 | 1:80:B:ALA:HA   | 9        | 0.1           |
| (1,94)  | 1:75:A:VAL:HG13 | 1:80:B:ALA:HA   | 9        | 0.1           |
| (1,87)  | 1:3:A:GLU:HG2   | 1:10:B:THR:HG21 | 16       | 0.1           |
| (1,87)  | 1:3:A:GLU:HG2   | 1:10:B:THR:HG22 | 16       | 0.1           |
| (1,87)  | 1:3:A:GLU:HG2   | 1:10:B:THR:HG23 | 16       | 0.1           |
| (1,82)  | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB1  | 2        | 0.1           |
| (1,82)  | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB2  | 2        | 0.1           |
| (1,82)  | 1:72:A:GLN:HB2  | 1:80:B:ALA:HB3  | 2        | 0.1           |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG21 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG22 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD21  | 1:14:B:VAL:HG23 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG21 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG22 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD22  | 1:14:B:VAL:HG23 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG21 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG22 | 10       | 0.1           |
| (1,75)  | 1:4:A:LEU:HD23  | 1:14:B:VAL:HG23 | 10       | 0.1           |
| (1,63)  | 1:71:A:PHE:HB2  | 1:82:B:THR:HG21 | 5        | 0.1           |
| (1,63)  | 1:71:A:PHE:HB2  | 1:82:B:THR:HG22 | 5        | 0.1           |
| (1,63)  | 1:71:A:PHE:HB2  | 1:82:B:THR:HG23 | 5        | 0.1           |
| (1,39)  | 1:4:A:LEU:HD21  | 1:40:B:GLU:HA   | 10       | 0.1           |
| (1,39)  | 1:4:A:LEU:HD22  | 1:40:B:GLU:HA   | 10       | 0.1           |
| (1,39)  | 1:4:A:LEU:HD23  | 1:40:B:GLU:HA   | 10       | 0.1           |

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

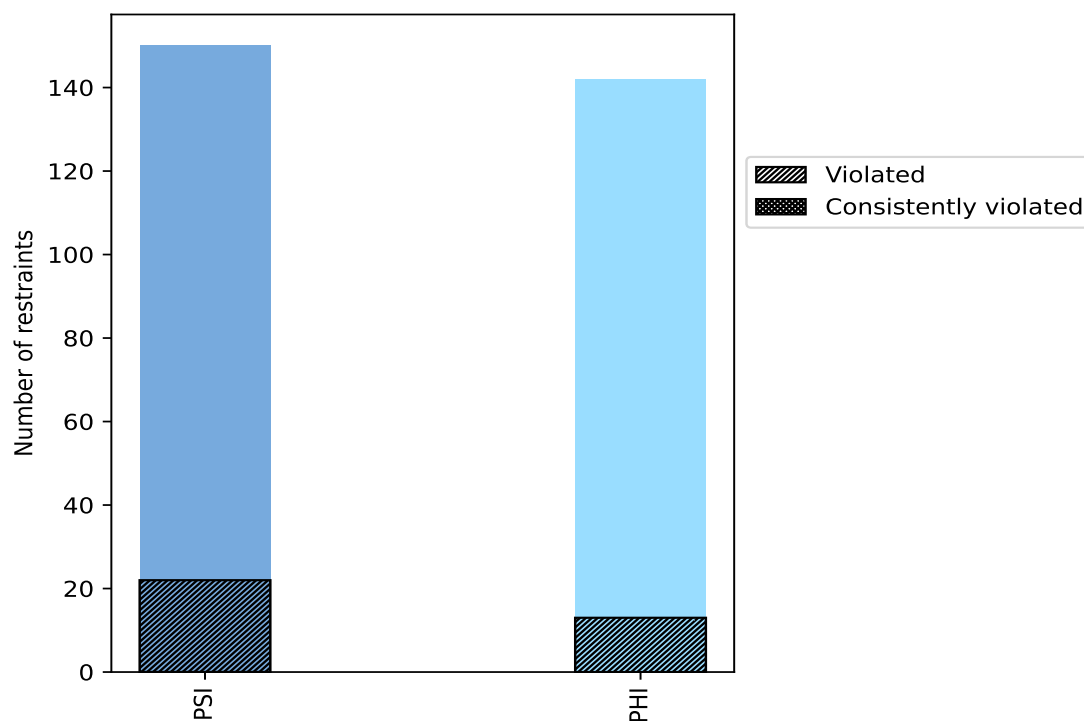
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 150   | 51.4           | 22                    | 14.7           | 7.5            | 0                                  | 0.0            | 0.0            |
| PHI        | 142   | 48.6           | 13                    | 9.2            | 4.5            | 0                                  | 0.0            | 0.0            |
| Total      | 292   | 100.0          | 35                    | 12.0           | 12.0           | 0                                  | 0.0            | 0.0            |

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

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



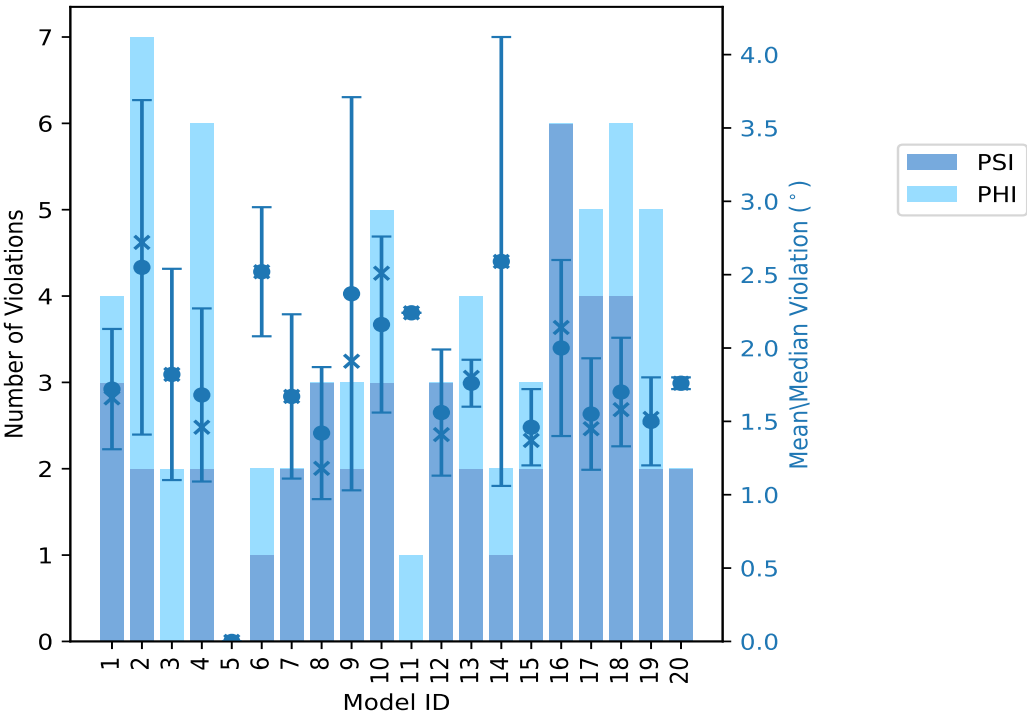
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 3                    | 1   | 4     | 1.72     | 2.31    | 0.41   | 1.66       |
| 2        | 2                    | 5   | 7     | 2.55     | 4.77    | 1.14   | 2.72       |
| 3        | 0                    | 2   | 2     | 1.82     | 2.54    | 0.72   | 1.82       |
| 4        | 2                    | 4   | 6     | 1.68     | 2.7     | 0.59   | 1.46       |
| 5        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 6        | 1                    | 1   | 2     | 2.52     | 2.96    | 0.44   | 2.52       |
| 7        | 2                    | 0   | 2     | 1.67     | 2.23    | 0.56   | 1.67       |
| 8        | 3                    | 0   | 3     | 1.42     | 2.06    | 0.45   | 1.18       |
| 9        | 2                    | 1   | 3     | 2.37     | 4.19    | 1.34   | 1.91       |
| 10       | 3                    | 2   | 5     | 2.16     | 2.73    | 0.6    | 2.51       |
| 11       | 0                    | 1   | 1     | 2.24     | 2.24    | 0.0    | 2.24       |
| 12       | 3                    | 0   | 3     | 1.56     | 2.14    | 0.43   | 1.41       |
| 13       | 2                    | 2   | 4     | 1.76     | 1.93    | 0.16   | 1.8        |
| 14       | 1                    | 1   | 2     | 2.59     | 4.12    | 1.53   | 2.59       |
| 15       | 2                    | 1   | 3     | 1.46     | 1.81    | 0.26   | 1.37       |
| 16       | 6                    | 0   | 6     | 2.0      | 2.85    | 0.6    | 2.14       |
| 17       | 4                    | 1   | 5     | 1.55     | 2.03    | 0.38   | 1.45       |
| 18       | 4                    | 2   | 6     | 1.7      | 2.37    | 0.37   | 1.58       |
| 19       | 2                    | 3   | 5     | 1.5      | 1.87    | 0.3    | 1.52       |
| 20       | 2                    | 0   | 2     | 1.76     | 1.8     | 0.04   | 1.76       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 12                            | 7   | 19    | 1                        | 5.0  |
| 5                             | 2   | 7     | 2                        | 10.0 |
| 3                             | 3   | 6     | 3                        | 15.0 |
| 1                             | 0   | 1     | 4                        | 20.0 |
| 0                             | 0   | 0     | 5                        | 25.0 |
| 0                             | 0   | 0     | 6                        | 30.0 |
| 0                             | 1   | 1     | 7                        | 35.0 |
| 0                             | 0   | 0     | 8                        | 40.0 |
| 1                             | 0   | 1     | 9                        | 45.0 |
| 0                             | 0   | 0     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

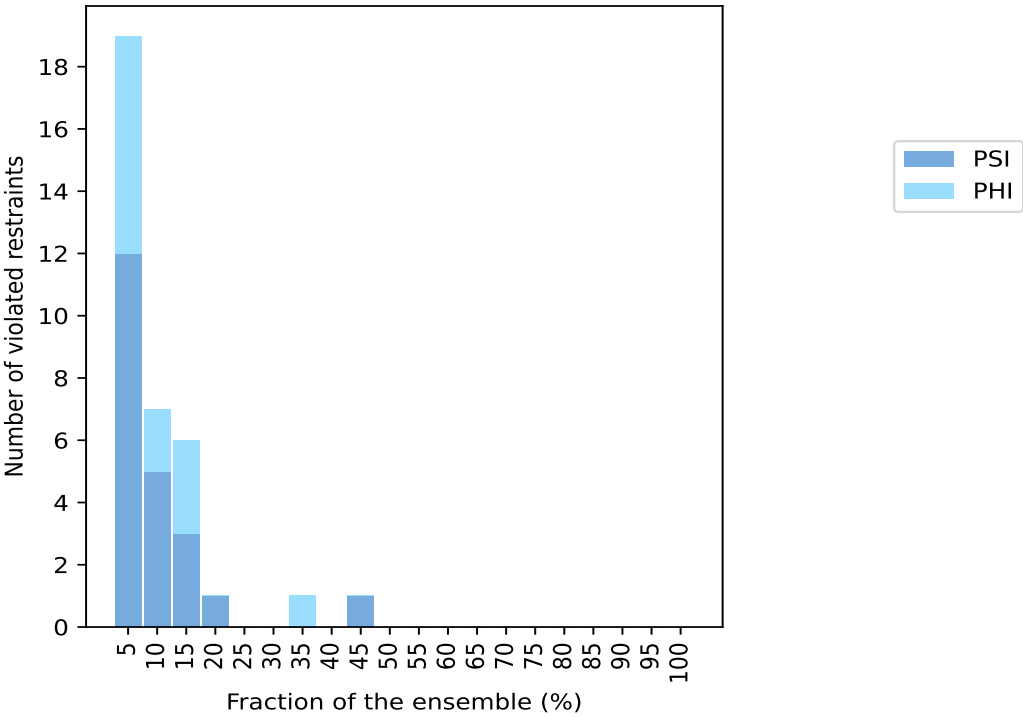
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

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

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

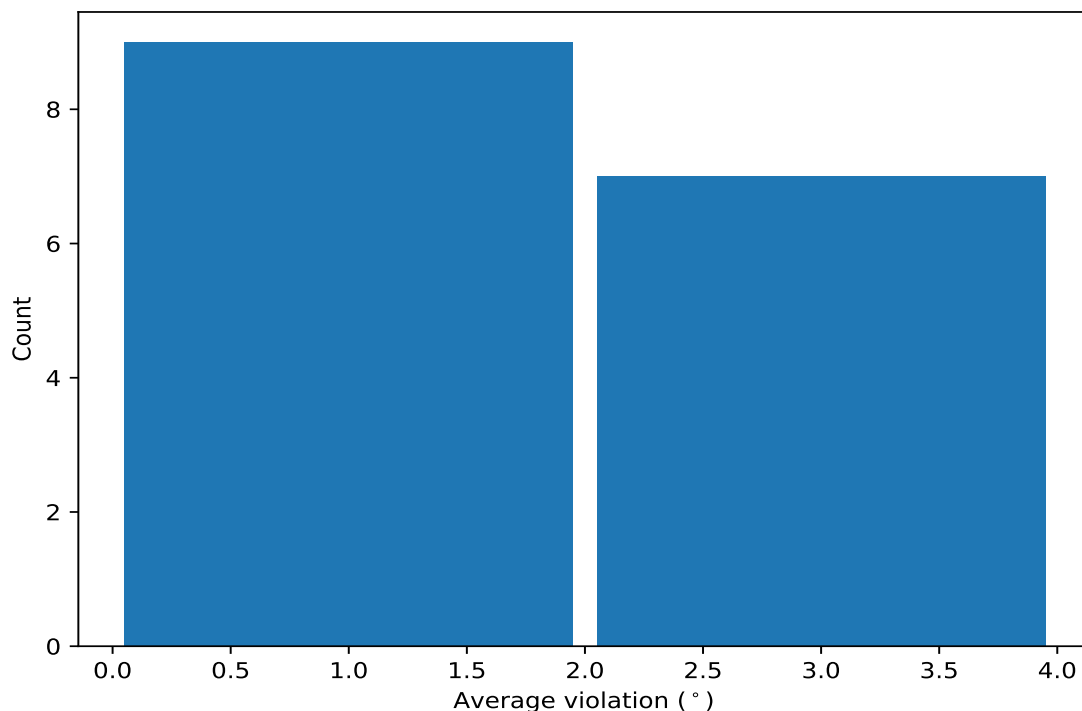


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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.

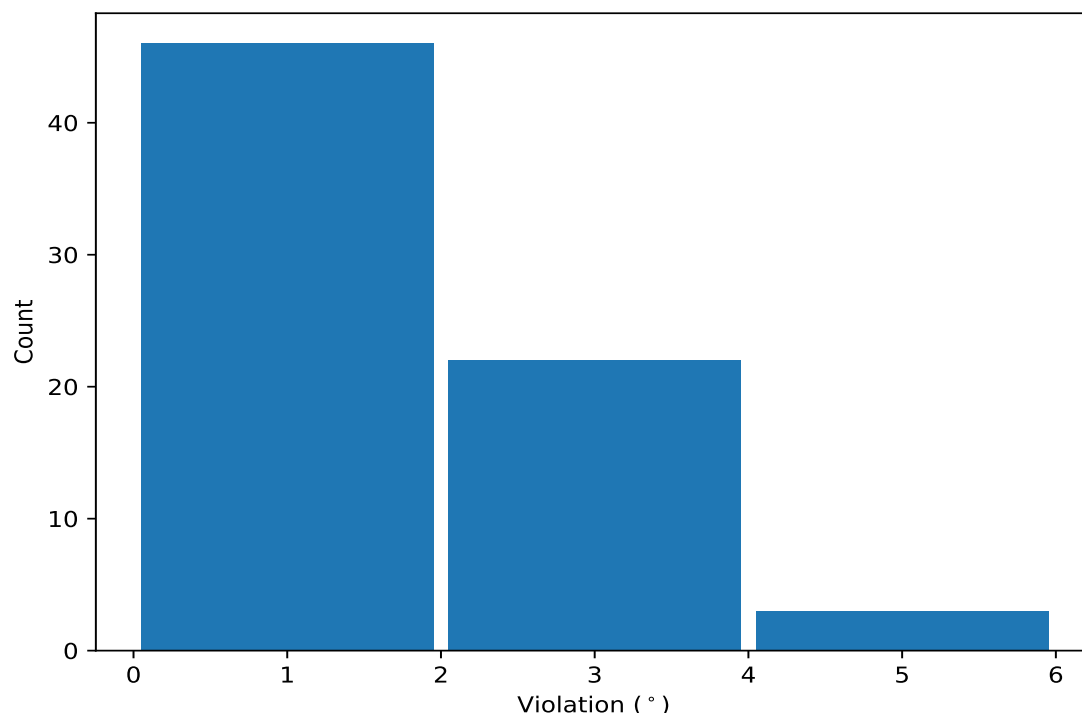
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 9                   | 1.65 | 0.91            | 1.28   |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 7                   | 2.31 | 0.92            | 2.24   |
| (1,269) | 1:68:B:GLU:N | 1:68:B:GLU:CA | 1:68:B:GLU:C  | 1:69:B:VAL:N | 4                   | 1.66 | 0.48            | 1.56   |
| (1,70)  | 1:90:A:TRP:C | 1:91:A:GLU:N  | 1:91:A:GLU:CA | 1:91:A:GLU:C | 3                   | 2.26 | 0.84            | 2.75   |
| (1,255) | 1:50:B:ASP:N | 1:50:B:ASP:CA | 1:50:B:ASP:C  | 1:51:B:VAL:N | 3                   | 2.15 | 0.41            | 1.91   |
| (1,165) | 1:27:B:LYS:C | 1:28:B:LEU:N  | 1:28:B:LEU:CA | 1:28:B:LEU:C | 3                   | 2.08 | 0.45            | 1.78   |
| (1,292) | 1:92:B:ASN:N | 1:92:B:ASN:CA | 1:92:B:ASN:C  | 1:93:B:SER:N | 3                   | 1.95 | 0.37            | 2.01   |
| (1,95)  | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C  | 1:30:A:LYS:N | 3                   | 1.69 | 0.38            | 1.72   |
| (1,48)  | 1:67:A:GLY:C | 1:68:A:GLU:N  | 1:68:A:GLU:CA | 1:68:A:GLU:C | 3                   | 1.39 | 0.41            | 1.11   |
| (1,217) | 1:91:B:GLU:C | 1:92:B:ASN:N  | 1:92:B:ASN:CA | 1:92:B:ASN:C | 2                   | 3.51 | 1.26            | 3.51   |
| (1,71)  | 1:91:A:GLU:C | 1:92:A:ASN:N  | 1:92:A:ASN:CA | 1:92:A:ASN:C | 2                   | 2.86 | 0.35            | 2.86   |
| (1,93)  | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C  | 1:28:A:LEU:N | 2                   | 2.35 | 0.5             | 2.35   |
| (1,102) | 1:41:A:LEU:N | 1:41:A:LEU:CA | 1:41:A:LEU:C  | 1:42:A:SER:N | 2                   | 1.7  | 0.36            | 1.7    |
| (1,120) | 1:64:A:ASN:N | 1:64:A:ASN:CA | 1:64:A:ASN:C  | 1:65:A:GLY:N | 2                   | 1.54 | 0.09            | 1.54   |
| (1,72)  | 1:2:A:SER:N  | 1:2:A:SER:CA  | 1:2:A:SER:C   | 1:3:A:GLU:N  | 2                   | 1.5  | 0.1             | 1.5    |
| (1,270) | 1:69:B:VAL:N | 1:69:B:VAL:CA | 1:69:B:VAL:C  | 1:70:B:ASP:N | 2                   | 1.49 | 0.31            | 1.49   |

<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 (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,217) | 1:91:B:GLU:C | 1:92:B:ASN:N  | 1:92:B:ASN:CA | 1:92:B:ASN:C | 2        | 4.77          |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 9        | 4.19          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 14       | 4.12          |
| (1,71)  | 1:91:A:GLU:C | 1:92:A:ASN:N  | 1:92:A:ASN:CA | 1:92:A:ASN:C | 2        | 3.2           |
| (1,70)  | 1:90:A:TRP:C | 1:91:A:GLU:N  | 1:91:A:GLU:CA | 1:91:A:GLU:C | 6        | 2.96          |
| (1,93)  | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C  | 1:28:A:LEU:N | 16       | 2.85          |
| (1,70)  | 1:90:A:TRP:C | 1:91:A:GLU:N  | 1:91:A:GLU:CA | 1:91:A:GLU:C | 2        | 2.75          |
| (1,255) | 1:50:B:ASP:N | 1:50:B:ASP:CA | 1:50:B:ASP:C  | 1:51:B:VAL:N | 10       | 2.73          |
| (1,165) | 1:27:B:LYS:C | 1:28:B:LEU:N  | 1:28:B:LEU:CA | 1:28:B:LEU:C | 2        | 2.72          |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 4        | 2.7           |
| (1,118) | 1:62:A:ASP:N | 1:62:A:ASP:CA | 1:62:A:ASP:C  | 1:63:A:GLU:N | 10       | 2.69          |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 3        | 2.54          |
| (1,71)  | 1:91:A:GLU:C | 1:92:A:ASN:N  | 1:92:A:ASN:CA | 1:92:A:ASN:C | 10       | 2.51          |
| (1,239) | 1:27:B:LYS:N | 1:27:B:LYS:CA | 1:27:B:LYS:C  | 1:28:B:LEU:N | 16       | 2.41          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,292) | 1:92:B:ASN:N | 1:92:B:ASN:CA | 1:92:B:ASN:C  | 1:93:B:SER:N | 18       | 2.37          |
| (1,269) | 1:68:B:GLU:N | 1:68:B:GLU:CA | 1:68:B:GLU:C  | 1:69:B:VAL:N | 1        | 2.31          |
| (1,92)  | 1:22:A:GLU:N | 1:22:A:GLU:CA | 1:22:A:GLU:C  | 1:23:A:GLY:N | 16       | 2.28          |
| (1,217) | 1:91:B:GLU:C | 1:92:B:ASN:N  | 1:92:B:ASN:CA | 1:92:B:ASN:C | 4        | 2.25          |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 11       | 2.24          |
| (1,267) | 1:65:B:GLY:N | 1:65:B:GLY:CA | 1:65:B:GLY:C  | 1:66:B:ASP:N | 7        | 2.23          |
| (1,95)  | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C  | 1:30:A:LYS:N | 12       | 2.14          |
| (1,123) | 1:68:A:GLU:N | 1:68:A:GLU:CA | 1:68:A:GLU:C  | 1:69:A:VAL:N | 6        | 2.08          |
| (1,102) | 1:41:A:LEU:N | 1:41:A:LEU:CA | 1:41:A:LEU:C  | 1:42:A:SER:N | 8        | 2.06          |
| (1,238) | 1:22:B:GLU:N | 1:22:B:GLU:CA | 1:22:B:GLU:C  | 1:23:B:GLY:N | 17       | 2.03          |
| (1,292) | 1:92:B:ASN:N | 1:92:B:ASN:CA | 1:92:B:ASN:C  | 1:93:B:SER:N | 16       | 2.01          |
| (1,48)  | 1:67:A:GLY:C | 1:68:A:GLU:N  | 1:68:A:GLU:CA | 1:68:A:GLU:C | 18       | 1.97          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 17       | 1.95          |
| (1,269) | 1:68:B:GLU:N | 1:68:B:GLU:CA | 1:68:B:GLU:C  | 1:69:B:VAL:N | 13       | 1.93          |
| (1,255) | 1:50:B:ASP:N | 1:50:B:ASP:CA | 1:50:B:ASP:C  | 1:51:B:VAL:N | 9        | 1.91          |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 19       | 1.87          |
| (1,193) | 1:66:B:ASP:C | 1:67:B:GLY:N  | 1:67:B:GLY:CA | 1:67:B:GLY:C | 1        | 1.85          |
| (1,93)  | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C  | 1:28:A:LEU:N | 13       | 1.85          |
| (1,255) | 1:50:B:ASP:N | 1:50:B:ASP:CA | 1:50:B:ASP:C  | 1:51:B:VAL:N | 15       | 1.81          |
| (1,270) | 1:69:B:VAL:N | 1:69:B:VAL:CA | 1:69:B:VAL:C  | 1:70:B:ASP:N | 20       | 1.8           |
| (1,165) | 1:27:B:LYS:C | 1:28:B:LEU:N  | 1:28:B:LEU:CA | 1:28:B:LEU:C | 19       | 1.78          |
| (1,165) | 1:27:B:LYS:C | 1:28:B:LEU:N  | 1:28:B:LEU:CA | 1:28:B:LEU:C | 13       | 1.74          |
| (1,109) | 1:50:A:ASP:N | 1:50:A:ASP:CA | 1:50:A:ASP:C  | 1:51:A:VAL:N | 18       | 1.72          |
| (1,95)  | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C  | 1:30:A:LYS:N | 20       | 1.72          |
| (1,120) | 1:64:A:ASN:N | 1:64:A:ASN:CA | 1:64:A:ASN:C  | 1:65:A:GLY:N | 10       | 1.64          |
| (1,72)  | 1:2:A:SER:N  | 1:2:A:SER:CA  | 1:2:A:SER:C   | 1:3:A:GLU:N  | 2        | 1.6           |
| (1,124) | 1:69:A:VAL:N | 1:69:A:VAL:CA | 1:69:A:VAL:C  | 1:70:A:ASP:N | 4        | 1.59          |
| (1,216) | 1:90:B:TRP:C | 1:91:B:GLU:N  | 1:91:B:GLU:CA | 1:91:B:GLU:C | 2        | 1.52          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 19       | 1.52          |
| (1,196) | 1:69:B:VAL:C | 1:70:B:ASP:N  | 1:70:B:ASP:CA | 1:70:B:ASP:C | 13       | 1.51          |
| (1,292) | 1:92:B:ASN:N | 1:92:B:ASN:CA | 1:92:B:ASN:C  | 1:93:B:SER:N | 1        | 1.47          |
| (1,120) | 1:64:A:ASN:N | 1:64:A:ASN:CA | 1:64:A:ASN:C  | 1:65:A:GLY:N | 17       | 1.45          |
| (1,36)  | 1:49:A:LYS:C | 1:50:A:ASP:N  | 1:50:A:ASP:CA | 1:50:A:ASP:C | 18       | 1.43          |
| (1,72)  | 1:2:A:SER:N  | 1:2:A:SER:CA  | 1:2:A:SER:C   | 1:3:A:GLU:N  | 12       | 1.41          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 18       | 1.38          |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 15       | 1.37          |
| (1,102) | 1:41:A:LEU:N | 1:41:A:LEU:CA | 1:41:A:LEU:C  | 1:42:A:SER:N | 18       | 1.34          |
| (1,194) | 1:67:B:GLY:C | 1:68:B:GLU:N  | 1:68:B:GLU:CA | 1:68:B:GLU:C | 4        | 1.32          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 16       | 1.28          |
| (1,266) | 1:64:B:ASN:N | 1:64:B:ASN:CA | 1:64:B:ASN:C  | 1:65:B:GLY:N | 2        | 1.26          |
| (1,19)  | 1:27:A:LYS:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 10       | 1.25          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 1        | 1.24          |
| (1,121) | 1:65:A:GLY:N | 1:65:A:GLY:CA | 1:65:A:GLY:C  | 1:66:A:ASP:N | 17       | 1.23          |
| (1,269) | 1:68:B:GLU:N | 1:68:B:GLU:CA | 1:68:B:GLU:C  | 1:69:B:VAL:N | 15       | 1.2           |
| (1,95)  | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C  | 1:30:A:LYS:N | 19       | 1.2           |
| (1,270) | 1:69:B:VAL:N | 1:69:B:VAL:CA | 1:69:B:VAL:C  | 1:70:B:ASP:N | 16       | 1.18          |
| (1,269) | 1:68:B:GLU:N | 1:68:B:GLU:CA | 1:68:B:GLU:C  | 1:69:B:VAL:N | 8        | 1.18          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 4        | 1.17          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 12       | 1.13          |
| (1,248) | 1:41:B:LEU:N | 1:41:B:LEU:CA | 1:41:B:LEU:C  | 1:42:B:SER:N | 7        | 1.11          |
| (1,48)  | 1:67:A:GLY:C | 1:68:A:GLU:N  | 1:68:A:GLU:CA | 1:68:A:GLU:C | 19       | 1.11          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,48)  | 1:67:A:GLY:C | 1:68:A:GLU:N  | 1:68:A:GLU:CA | 1:68:A:GLU:C | 17       | 1.1           |
| (1,174) | 1:39:B:THR:C | 1:40:B:GLU:N  | 1:40:B:GLU:CA | 1:40:B:GLU:C | 3        | 1.09          |
| (1,70)  | 1:90:A:TRP:C | 1:91:A:GLU:N  | 1:91:A:GLU:CA | 1:91:A:GLU:C | 4        | 1.08          |
| (1,163) | 1:17:B:ALA:C | 1:18:B:HIS:N  | 1:18:B:HIS:CA | 1:18:B:HIS:C | 14       | 1.06          |
| (1,146) | 1:92:A:ASN:N | 1:92:A:ASN:CA | 1:92:A:ASN:C  | 1:93:A:SER:N | 8        | 1.03          |
| (1,240) | 1:28:B:LEU:N | 1:28:B:LEU:CA | 1:28:B:LEU:C  | 1:29:B:SER:N | 9        | 1.01          |