



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:54 PM UTC

PDB ID : 6YW8 / pdb\_00006yw8  
BMRB ID : 34515  
Title : NMR solution structure of unbound recombinant human Nerve Growth Factor (rhNGF)  
Authors : Golic Grdadolnik, S.; Paoletti, F.  
Deposited on : 2020-04-29

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

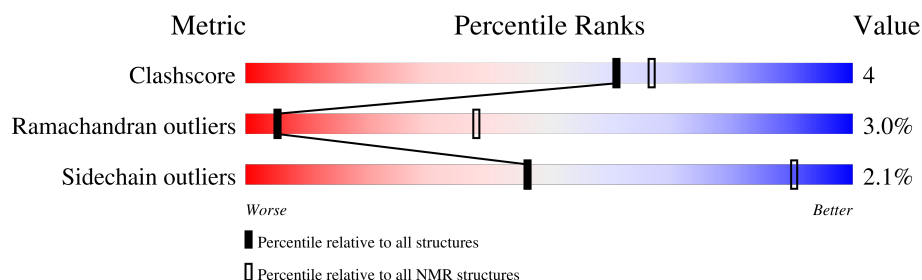
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 39%.

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     | 118    |                  |
| 1   | B     | 118    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:10-A:114, B:10-B:114<br>(210) | 1.91              | 1            |

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3680 atoms, of which 1820 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-nerve growth factor.

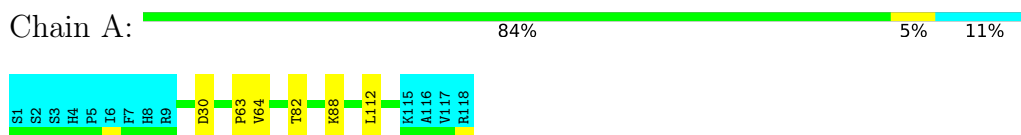
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 118      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1840  | 583 | 910 | 166 | 173 | 8 |       |
| 1   | B     | 118      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1840  | 583 | 910 | 166 | 173 | 8 |       |

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

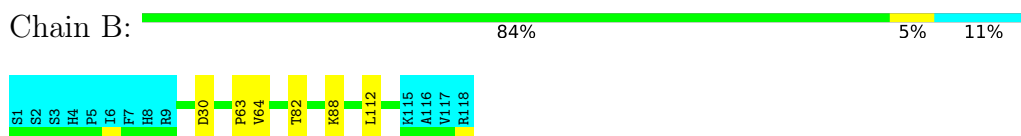
### 4.1 Average score per residue in the NMR ensemble

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: Beta-nerve growth factor



- Molecule 1: Beta-nerve growth factor

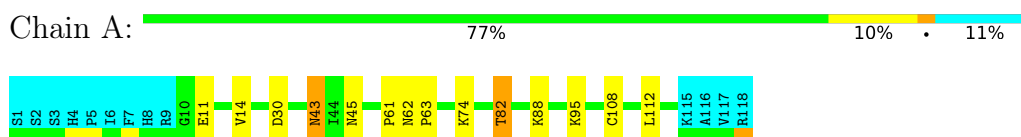


### 4.2 Scores per residue for each member of the ensemble

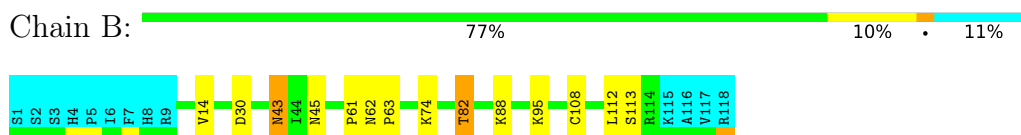
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Beta-nerve growth factor

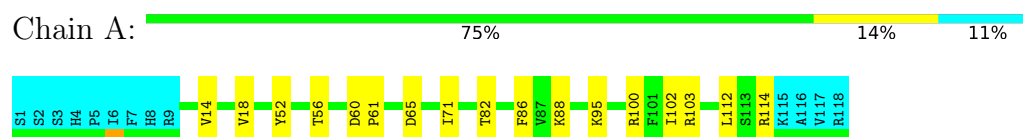


- Molecule 1: Beta-nerve growth factor

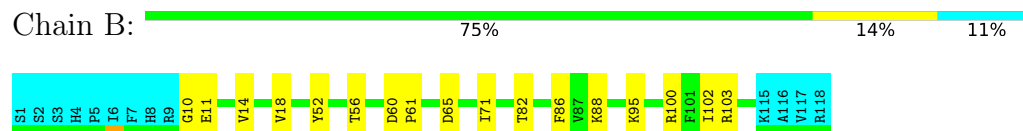


### 4.2.2 Score per residue for model 2

- Molecule 1: Beta-nerve growth factor

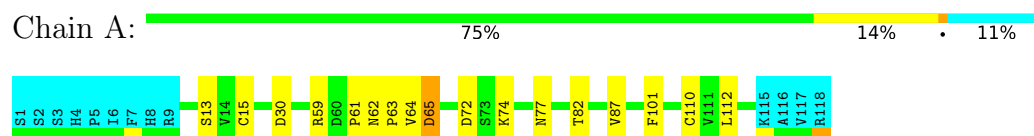


- Molecule 1: Beta-nerve growth factor

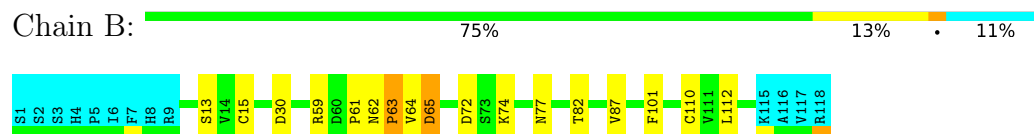


### 4.2.3 Score per residue for model 3

- Molecule 1: Beta-nerve growth factor

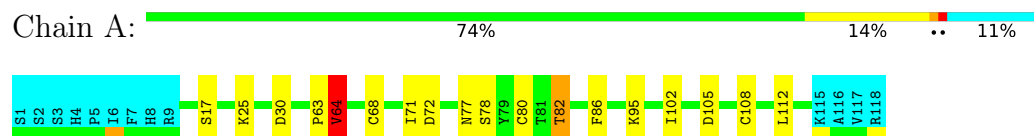


- Molecule 1: Beta-nerve growth factor

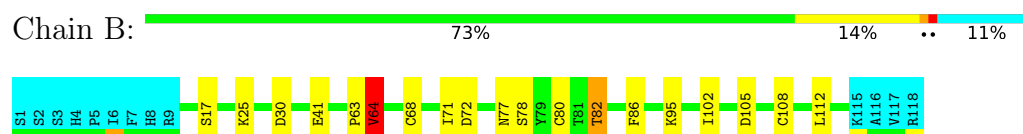


### 4.2.4 Score per residue for model 4

- Molecule 1: Beta-nerve growth factor



- Molecule 1: Beta-nerve growth factor



### 4.2.5 Score per residue for model 5

- Molecule 1: Beta-nerve growth factor

Chain A:  76% 13% 11%



- Molecule 1: Beta-nerve growth factor

Chain B:  76% 13% 11%



### 4.2.6 Score per residue for model 6

- Molecule 1: Beta-nerve growth factor

Chain A:  77% 12% 11%



- Molecule 1: Beta-nerve growth factor

Chain B:  75% 14% 11%



### 4.2.7 Score per residue for model 7

- Molecule 1: Beta-nerve growth factor

Chain A:  74% 14% 11%



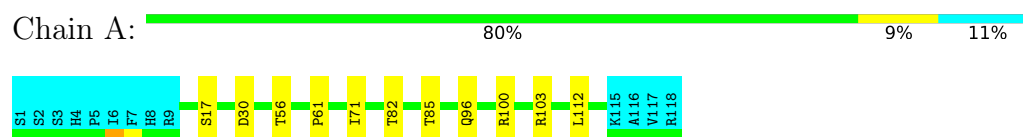
- Molecule 1: Beta-nerve growth factor

Chain B:  74% 14% 11%

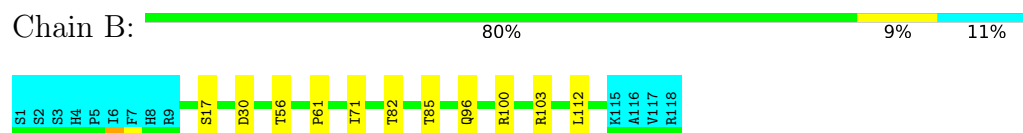


### 4.2.8 Score per residue for model 8

- Molecule 1: Beta-nerve growth factor

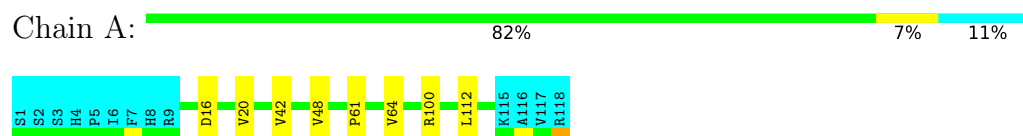


- Molecule 1: Beta-nerve growth factor

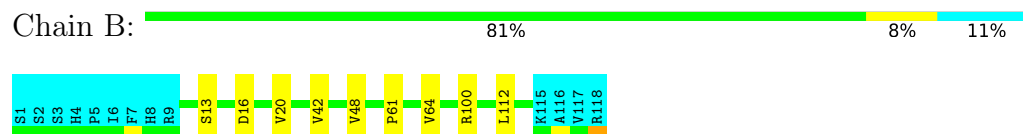


### 4.2.9 Score per residue for model 9

- Molecule 1: Beta-nerve growth factor

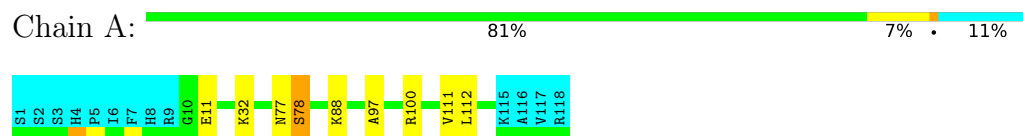


- Molecule 1: Beta-nerve growth factor

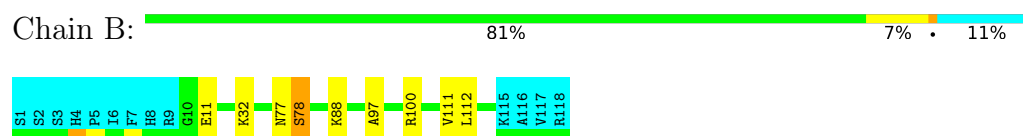


### 4.2.10 Score per residue for model 10

- Molecule 1: Beta-nerve growth factor



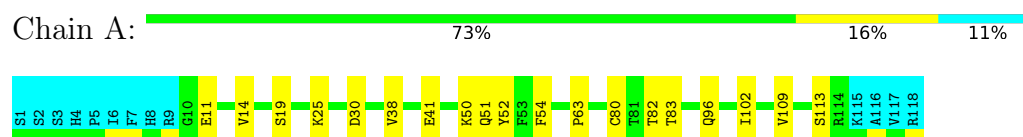
- Molecule 1: Beta-nerve growth factor



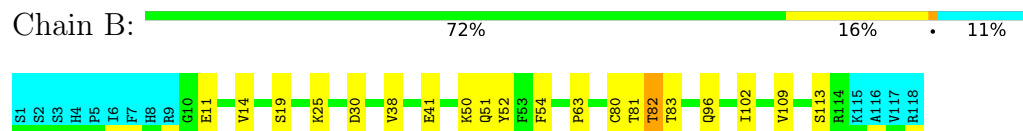


### 4.2.11 Score per residue for model 11

- Molecule 1: Beta-nerve growth factor

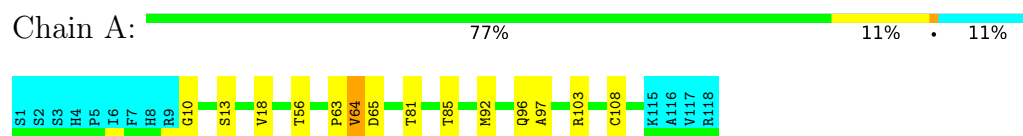


- Molecule 1: Beta-nerve growth factor

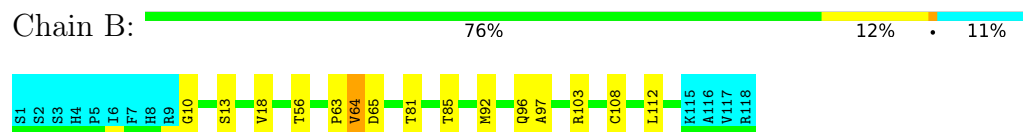


### 4.2.12 Score per residue for model 12

- Molecule 1: Beta-nerve growth factor

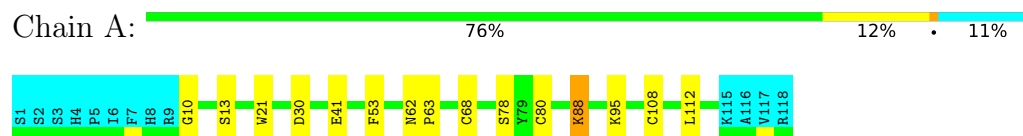


- Molecule 1: Beta-nerve growth factor

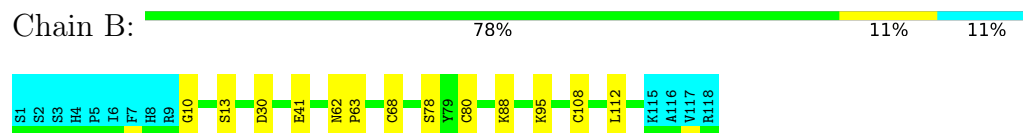


### 4.2.13 Score per residue for model 13

- Molecule 1: Beta-nerve growth factor

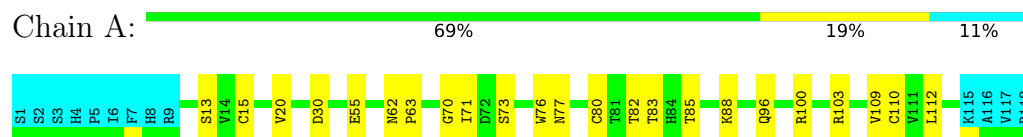


- Molecule 1: Beta-nerve growth factor

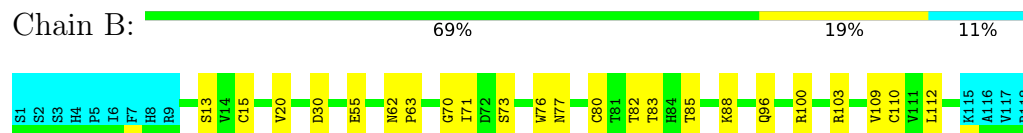


#### 4.2.14 Score per residue for model 14

- Molecule 1: Beta-nerve growth factor

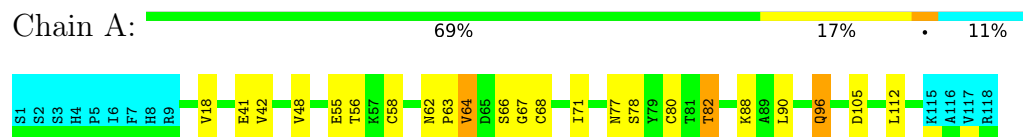


- Molecule 1: Beta-nerve growth factor

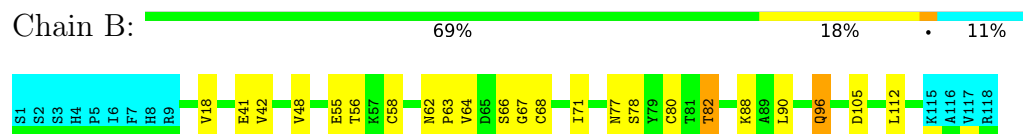


#### 4.2.15 Score per residue for model 15

- Molecule 1: Beta-nerve growth factor

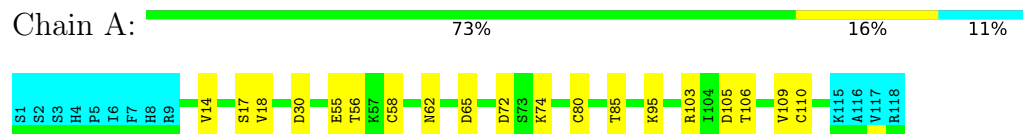


- Molecule 1: Beta-nerve growth factor

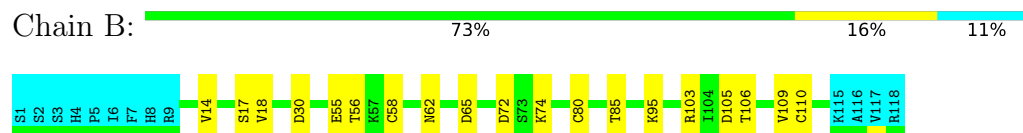


#### 4.2.16 Score per residue for model 16

- Molecule 1: Beta-nerve growth factor



- Molecule 1: Beta-nerve growth factor



### 4.2.17 Score per residue for model 17

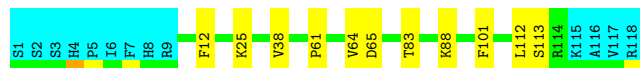
- Molecule 1: Beta-nerve growth factor

Chain A: 



- Molecule 1: Beta-nerve growth factor

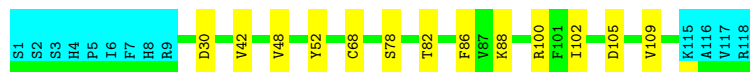
Chain B: 



### 4.2.18 Score per residue for model 18

- Molecule 1: Beta-nerve growth factor

Chain A: 



- Molecule 1: Beta-nerve growth factor

Chain B: 



### 4.2.19 Score per residue for model 19

- Molecule 1: Beta-nerve growth factor

Chain A: 



- Molecule 1: Beta-nerve growth factor

Chain B: 



#### 4.2.20 Score per residue for model 20

- Molecule 1: Beta-nerve growth factor

Chain A:  75% 13% • 11%



- Molecule 1: Beta-nerve growth factor

Chain B:  75% 14% • 11%



## 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 |
|---------------|-----------------------|---------|
| ARIA          | refinement            | 2.3.2   |
| ARIA          | structure calculation | 2.3.2   |

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                       | 1208           |
| Number of shifts mapped to atoms             | 1208           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 39%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 822   | 797      | 795      | 8±2     |
| 1   | B     | 822   | 797      | 795      | 8±2     |
| All | All   | 32880 | 31880    | 31800    | 287     |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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

| Atom-1         | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|----------------|------------------|----------|-------------|--------|-------|
|                |                  |          |             | Worst  | Total |
| 1:A:77:ASN:O   | 1:A:78:SER:HB2   | 0.62     | 1.95        | 10     | 1     |
| 1:B:77:ASN:O   | 1:B:78:SER:HB2   | 0.61     | 1.95        | 10     | 1     |
| 1:B:68:CYS:SG  | 1:B:78:SER:HB3   | 0.59     | 2.36        | 5      | 2     |
| 1:A:88:LYS:N   | 1:A:88:LYS:HD2   | 0.59     | 2.12        | 18     | 10    |
| 1:B:88:LYS:N   | 1:B:88:LYS:HD2   | 0.59     | 2.12        | 2      | 9     |
| 1:A:68:CYS:SG  | 1:A:78:SER:HB3   | 0.58     | 2.37        | 5      | 2     |
| 1:B:55:GLU:HA  | 1:B:105:ASP:O    | 0.58     | 1.98        | 19     | 4     |
| 1:A:55:GLU:HA  | 1:A:105:ASP:O    | 0.58     | 1.99        | 19     | 4     |
| 1:B:88:LYS:HD2 | 1:B:88:LYS:N     | 0.58     | 2.13        | 15     | 1     |
| 1:B:62:ASN:N   | 1:B:63:PRO:HD3   | 0.57     | 2.13        | 5      | 3     |
| 1:A:62:ASN:N   | 1:A:63:PRO:HD3   | 0.57     | 2.14        | 5      | 3     |
| 1:B:112:LEU:H  | 1:B:112:LEU:HD23 | 0.57     | 1.60        | 19     | 12    |
| 1:A:112:LEU:H  | 1:A:112:LEU:HD23 | 0.57     | 1.60        | 19     | 12    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:68:CYS:SG   | 1:A:78:SER:HB2  | 0.56     | 2.41        | 18     | 3     |
| 1:B:68:CYS:SG   | 1:B:78:SER:HB2  | 0.56     | 2.40        | 18     | 3     |
| 1:A:80:CYS:SG   | 1:A:108:CYS:HB3 | 0.55     | 2.42        | 7      | 2     |
| 1:B:80:CYS:SG   | 1:B:108:CYS:HB3 | 0.55     | 2.42        | 7      | 2     |
| 1:A:30:ASP:OD2  | 1:A:100:ARG:HB3 | 0.54     | 2.03        | 8      | 2     |
| 1:B:30:ASP:OD2  | 1:B:100:ARG:HB3 | 0.53     | 2.04        | 8      | 2     |
| 1:A:78:SER:HB3  | 1:A:111:VAL:O   | 0.53     | 2.04        | 10     | 1     |
| 1:B:78:SER:HB3  | 1:B:111:VAL:O   | 0.52     | 2.04        | 10     | 1     |
| 1:A:96:GLN:HE21 | 1:A:96:GLN:N    | 0.52     | 2.02        | 15     | 1     |
| 1:B:96:GLN:HE21 | 1:B:96:GLN:N    | 0.52     | 2.02        | 15     | 1     |
| 1:B:82:THR:HG23 | 1:B:108:CYS:SG  | 0.52     | 2.45        | 4      | 2     |
| 1:A:82:THR:HG23 | 1:A:108:CYS:SG  | 0.52     | 2.45        | 4      | 2     |
| 1:A:110:CYS:O   | 1:B:110:CYS:HB2 | 0.51     | 2.05        | 16     | 1     |
| 1:B:18:VAL:O    | 1:B:56:THR:HA   | 0.51     | 2.05        | 16     | 4     |
| 1:B:25:LYS:O    | 1:B:38:VAL:HB   | 0.51     | 2.06        | 7      | 3     |
| 1:A:18:VAL:O    | 1:A:56:THR:HA   | 0.51     | 2.04        | 16     | 4     |
| 1:A:63:PRO:O    | 1:A:64:VAL:HG22 | 0.51     | 2.06        | 4      | 3     |
| 1:A:25:LYS:O    | 1:A:38:VAL:HB   | 0.51     | 2.06        | 7      | 3     |
| 1:A:42:VAL:O    | 1:A:48:VAL:HA   | 0.50     | 2.07        | 15     | 3     |
| 1:B:42:VAL:O    | 1:B:48:VAL:HA   | 0.50     | 2.07        | 15     | 3     |
| 1:B:63:PRO:O    | 1:B:64:VAL:HG22 | 0.50     | 2.07        | 4      | 2     |
| 1:A:60:ASP:N    | 1:A:61:PRO:HD3  | 0.50     | 2.22        | 20     | 2     |
| 1:B:60:ASP:N    | 1:B:61:PRO:HD3  | 0.50     | 2.22        | 20     | 2     |
| 1:A:110:CYS:HB2 | 1:B:110:CYS:O   | 0.49     | 2.07        | 16     | 1     |
| 1:B:88:LYS:HA   | 1:B:100:ARG:O   | 0.49     | 2.08        | 6      | 4     |
| 1:A:88:LYS:HA   | 1:A:100:ARG:O   | 0.49     | 2.08        | 6      | 4     |
| 1:B:100:ARG:HA  | 1:B:100:ARG:NE  | 0.49     | 2.23        | 2      | 6     |
| 1:B:61:PRO:O    | 1:B:64:VAL:HG22 | 0.49     | 2.07        | 9      | 1     |
| 1:A:100:ARG:HA  | 1:A:100:ARG:NE  | 0.48     | 2.23        | 2      | 6     |
| 1:A:15:CYS:HB2  | 1:A:110:CYS:SG  | 0.48     | 2.48        | 3      | 2     |
| 1:A:61:PRO:O    | 1:A:64:VAL:HG22 | 0.48     | 2.08        | 9      | 1     |
| 1:A:72:ASP:O    | 1:A:74:LYS:HD2  | 0.48     | 2.08        | 16     | 2     |
| 1:A:19:SER:HA   | 1:A:55:GLU:O    | 0.48     | 2.09        | 20     | 1     |
| 1:A:88:LYS:HE3  | 1:A:101:PHE:CD1 | 0.48     | 2.43        | 5      | 2     |
| 1:A:80:CYS:HB3  | 1:A:108:CYS:SG  | 0.48     | 2.49        | 13     | 1     |
| 1:A:70:GLY:O    | 1:B:71:ILE:HA   | 0.48     | 2.09        | 14     | 1     |
| 1:A:71:ILE:HA   | 1:B:70:GLY:O    | 0.48     | 2.09        | 14     | 1     |
| 1:B:15:CYS:HB2  | 1:B:110:CYS:SG  | 0.47     | 2.49        | 3      | 2     |
| 1:B:19:SER:HA   | 1:B:55:GLU:O    | 0.47     | 2.09        | 20     | 1     |
| 1:A:80:CYS:HA   | 1:A:109:VAL:O   | 0.47     | 2.09        | 11     | 3     |
| 1:B:66:SER:O    | 1:B:78:SER:HB3  | 0.47     | 2.09        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:109:VAL:HG12 | 1:B:109:VAL:HG12 | 0.47     | 1.85        | 6      | 1     |
| 1:B:112:LEU:O    | 1:B:112:LEU:HG   | 0.47     | 2.09        | 19     | 4     |
| 1:A:66:SER:O     | 1:A:78:SER:HB3   | 0.47     | 2.09        | 20     | 1     |
| 1:B:80:CYS:HB3   | 1:B:108:CYS:SG   | 0.47     | 2.49        | 13     | 1     |
| 1:B:72:ASP:O     | 1:B:74:LYS:HD2   | 0.47     | 2.09        | 16     | 2     |
| 1:A:85:THR:O     | 1:A:103:ARG:HA   | 0.47     | 2.09        | 12     | 7     |
| 1:B:88:LYS:HE3   | 1:B:101:PHE:CD1  | 0.47     | 2.44        | 5      | 2     |
| 1:A:73:SER:H     | 1:A:76:TRP:CD1   | 0.47     | 2.27        | 14     | 1     |
| 1:B:73:SER:H     | 1:B:76:TRP:CD1   | 0.47     | 2.27        | 14     | 1     |
| 1:B:92:MET:HA    | 1:B:96:GLN:O     | 0.47     | 2.10        | 19     | 1     |
| 1:B:80:CYS:HA    | 1:B:109:VAL:O    | 0.47     | 2.10        | 11     | 3     |
| 1:A:11:GLU:H     | 1:A:11:GLU:CD    | 0.47     | 2.17        | 20     | 1     |
| 1:B:11:GLU:H     | 1:B:11:GLU:CD    | 0.47     | 2.17        | 20     | 1     |
| 1:A:112:LEU:O    | 1:A:112:LEU:HG   | 0.47     | 2.10        | 19     | 4     |
| 1:B:59:ARG:C     | 1:B:61:PRO:HD3   | 0.46     | 2.34        | 3      | 1     |
| 1:B:85:THR:O     | 1:B:103:ARG:HA   | 0.46     | 2.10        | 12     | 7     |
| 1:A:59:ARG:C     | 1:A:61:PRO:HD3   | 0.46     | 2.34        | 3      | 1     |
| 1:A:30:ASP:OD1   | 1:A:100:ARG:HB3  | 0.46     | 2.10        | 7      | 2     |
| 1:A:82:THR:CG2   | 1:A:105:ASP:HB3  | 0.46     | 2.41        | 4      | 4     |
| 1:A:109:VAL:HG21 | 1:B:109:VAL:HG11 | 0.46     | 1.87        | 11     | 1     |
| 1:A:109:VAL:HG11 | 1:B:109:VAL:HG11 | 0.46     | 1.87        | 18     | 1     |
| 1:B:82:THR:CG2   | 1:B:105:ASP:HB3  | 0.45     | 2.41        | 4      | 4     |
| 1:A:51:GLN:HA    | 1:A:51:GLN:OE1   | 0.45     | 2.10        | 11     | 1     |
| 1:A:20:VAL:HG22  | 1:A:55:GLU:O     | 0.45     | 2.11        | 14     | 1     |
| 1:A:82:THR:CG2   | 1:A:105:ASP:HB2  | 0.45     | 2.41        | 18     | 1     |
| 1:A:92:MET:HA    | 1:A:96:GLN:O     | 0.45     | 2.12        | 19     | 1     |
| 1:A:109:VAL:HG11 | 1:B:109:VAL:HG21 | 0.45     | 1.88        | 11     | 1     |
| 1:B:51:GLN:HA    | 1:B:51:GLN:OE1   | 0.45     | 2.10        | 11     | 1     |
| 1:A:58:CYS:SG    | 1:A:80:CYS:HB3   | 0.45     | 2.51        | 15     | 1     |
| 1:B:58:CYS:SG    | 1:B:80:CYS:HB3   | 0.45     | 2.51        | 15     | 1     |
| 1:B:20:VAL:HG22  | 1:B:55:GLU:O     | 0.45     | 2.12        | 14     | 1     |
| 1:B:82:THR:CG2   | 1:B:105:ASP:HB2  | 0.45     | 2.42        | 18     | 1     |
| 1:A:56:THR:HB    | 1:A:106:THR:O    | 0.45     | 2.11        | 16     | 1     |
| 1:A:62:ASN:N     | 1:A:63:PRO:CD    | 0.45     | 2.79        | 1      | 2     |
| 1:B:62:ASN:N     | 1:B:63:PRO:CD    | 0.45     | 2.79        | 1      | 2     |
| 1:B:30:ASP:OD1   | 1:B:100:ARG:HB3  | 0.45     | 2.11        | 7      | 3     |
| 1:B:17:SER:HB3   | 1:B:58:CYS:SG    | 0.45     | 2.52        | 16     | 2     |
| 1:A:113:SER:HA   | 1:B:12:PHE:CD2   | 0.45     | 2.47        | 17     | 1     |
| 1:B:56:THR:HB    | 1:B:106:THR:O    | 0.45     | 2.12        | 16     | 1     |
| 1:A:12:PHE:CD2   | 1:B:113:SER:HA   | 0.45     | 2.47        | 17     | 1     |
| 1:A:25:LYS:HB2   | 1:A:53:PHE:CE2   | 0.44     | 2.48        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:25:LYS:HB2   | 1:B:53:PHE:CE2   | 0.44     | 2.48        | 19     | 1     |
| 1:A:86:PHE:HA    | 1:A:102:ILE:O    | 0.44     | 2.13        | 18     | 3     |
| 1:B:86:PHE:HA    | 1:B:102:ILE:O    | 0.44     | 2.13        | 18     | 3     |
| 1:A:19:SER:HB3   | 1:A:54:PHE:CZ    | 0.44     | 2.47        | 11     | 1     |
| 1:A:17:SER:HB3   | 1:A:58:CYS:SG    | 0.44     | 2.53        | 16     | 2     |
| 1:B:103:ARG:HG3  | 1:B:103:ARG:O    | 0.44     | 2.12        | 2      | 1     |
| 1:B:19:SER:HB3   | 1:B:54:PHE:CZ    | 0.44     | 2.48        | 11     | 1     |
| 1:A:43:ASN:C     | 1:A:43:ASN:HD22  | 0.44     | 2.20        | 1      | 1     |
| 1:A:87:VAL:O     | 1:A:101:PHE:HA   | 0.43     | 2.13        | 3      | 1     |
| 1:A:62:ASN:N     | 1:A:63:PRO:HD2   | 0.43     | 2.28        | 15     | 1     |
| 1:B:62:ASN:N     | 1:B:63:PRO:HD2   | 0.43     | 2.28        | 15     | 1     |
| 1:B:43:ASN:C     | 1:B:43:ASN:HD22  | 0.43     | 2.20        | 1      | 1     |
| 1:B:87:VAL:O     | 1:B:101:PHE:HA   | 0.43     | 2.13        | 3      | 1     |
| 1:B:30:ASP:HA    | 1:B:102:ILE:HA   | 0.43     | 1.90        | 11     | 1     |
| 1:A:103:ARG:HG3  | 1:A:103:ARG:O    | 0.43     | 2.13        | 2      | 1     |
| 1:A:11:GLU:O     | 1:B:113:SER:HA   | 0.43     | 2.14        | 1      | 1     |
| 1:A:114:ARG:O    | 1:B:10:GLY:HA2   | 0.43     | 2.13        | 2      | 1     |
| 1:A:17:SER:HB3   | 1:A:108:CYS:SG   | 0.43     | 2.53        | 4      | 1     |
| 1:B:17:SER:HB3   | 1:B:108:CYS:SG   | 0.43     | 2.53        | 4      | 1     |
| 1:A:21:TRP:HB3   | 1:A:52:TYR:HB3   | 0.43     | 1.90        | 6      | 1     |
| 1:A:30:ASP:HA    | 1:A:102:ILE:HA   | 0.43     | 1.90        | 11     | 1     |
| 1:B:21:TRP:HB3   | 1:B:52:TYR:HB3   | 0.42     | 1.91        | 6      | 1     |
| 1:A:42:VAL:CG1   | 1:A:90:LEU:HB3   | 0.42     | 2.44        | 15     | 1     |
| 1:A:92:MET:SD    | 1:A:97:ALA:HB2   | 0.42     | 2.55        | 12     | 1     |
| 1:B:81:THR:O     | 1:B:108:CYS:HA   | 0.42     | 2.15        | 12     | 1     |
| 1:B:42:VAL:CG1   | 1:B:90:LEU:HB3   | 0.42     | 2.44        | 15     | 1     |
| 1:A:81:THR:O     | 1:A:108:CYS:HA   | 0.42     | 2.15        | 12     | 1     |
| 1:A:21:TRP:HA    | 1:A:53:PHE:O     | 0.42     | 2.14        | 20     | 2     |
| 1:B:92:MET:SD    | 1:B:97:ALA:HB2   | 0.42     | 2.55        | 12     | 1     |
| 1:B:21:TRP:HA    | 1:B:53:PHE:O     | 0.41     | 2.14        | 20     | 1     |
| 1:A:77:ASN:OD1   | 1:A:114:ARG:HD2  | 0.41     | 2.16        | 7      | 1     |
| 1:A:17:SER:HB2   | 1:A:56:THR:CG2   | 0.41     | 2.46        | 8      | 1     |
| 1:A:112:LEU:HD23 | 1:A:112:LEU:N    | 0.41     | 2.30        | 10     | 1     |
| 1:B:112:LEU:N    | 1:B:112:LEU:HD23 | 0.41     | 2.30        | 10     | 1     |
| 1:B:77:ASN:OD1   | 1:B:114:ARG:HD2  | 0.41     | 2.16        | 7      | 1     |
| 1:A:13:SER:O     | 1:A:63:PRO:HB2   | 0.41     | 2.16        | 3      | 1     |
| 1:A:112:LEU:O    | 1:B:11:GLU:HB3   | 0.41     | 2.16        | 2      | 1     |
| 1:B:13:SER:O     | 1:B:63:PRO:HB2   | 0.41     | 2.16        | 3      | 1     |
| 1:B:17:SER:HB2   | 1:B:56:THR:CG2   | 0.41     | 2.46        | 8      | 1     |
| 1:A:89:ALA:O     | 1:A:99:TRP:HA    | 0.40     | 2.15        | 5      | 1     |
| 1:B:81:THR:O     | 1:B:82:THR:HB    | 0.40     | 2.16        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:62:ASN:HB3   | 1:A:65:ASP:O     | 0.40     | 2.16        | 3      | 1     |
| 1:B:89:ALA:O     | 1:B:99:TRP:HA    | 0.40     | 2.15        | 5      | 1     |
| 1:A:112:LEU:HG   | 1:A:112:LEU:O    | 0.40     | 2.16        | 3      | 1     |
| 1:B:62:ASN:HB3   | 1:B:65:ASP:O     | 0.40     | 2.16        | 3      | 1     |
| 1:B:112:LEU:HG   | 1:B:112:LEU:O    | 0.40     | 2.16        | 3      | 1     |
| 1:B:84:HIS:HA    | 1:B:104:ILE:O    | 0.40     | 2.16        | 6      | 1     |
| 1:A:78:SER:OG    | 1:A:111:VAL:HG13 | 0.40     | 2.16        | 10     | 1     |
| 1:B:112:LEU:HD23 | 1:B:112:LEU:H    | 0.40     | 1.76        | 12     | 1     |
| 1:A:50:LYS:HE2   | 1:A:52:TYR:OH    | 0.40     | 2.16        | 19     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|------------|-------------|----|
| 1   | A     | 105/118 (89%)   | 89±3 (85±3%) | 13±3 (13±3%) | 3±1 (3±1%) | 5           | 39 |
| 1   | B     | 105/118 (89%)   | 89±3 (85±3%) | 13±3 (12±3%) | 3±1 (3±1%) | 5           | 38 |
| All | All   | 4200/4720 (89%) | 3553 (85%)   | 523 (12%)    | 124 (3%)   | 5           | 38 |

All 48 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 64  | VAL  | 6              |
| 1   | B     | 64  | VAL  | 6              |
| 1   | A     | 14  | VAL  | 5              |
| 1   | B     | 14  | VAL  | 5              |
| 1   | A     | 65  | ASP  | 5              |
| 1   | A     | 71  | ILE  | 5              |
| 1   | B     | 65  | ASP  | 5              |
| 1   | B     | 71  | ILE  | 5              |
| 1   | A     | 61  | PRO  | 4              |
| 1   | A     | 95  | LYS  | 4              |
| 1   | B     | 61  | PRO  | 4              |
| 1   | B     | 95  | LYS  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 82  | THR  | 4              |
| 1   | B     | 82  | THR  | 4              |
| 1   | B     | 13  | SER  | 4              |
| 1   | A     | 52  | TYR  | 3              |
| 1   | B     | 52  | TYR  | 3              |
| 1   | B     | 63  | PRO  | 3              |
| 1   | A     | 96  | GLN  | 3              |
| 1   | B     | 96  | GLN  | 3              |
| 1   | A     | 13  | SER  | 3              |
| 1   | A     | 45  | ASN  | 2              |
| 1   | B     | 45  | ASN  | 2              |
| 1   | A     | 66  | SER  | 2              |
| 1   | B     | 66  | SER  | 2              |
| 1   | A     | 63  | PRO  | 2              |
| 1   | A     | 83  | THR  | 2              |
| 1   | B     | 83  | THR  | 2              |
| 1   | A     | 10  | GLY  | 2              |
| 1   | B     | 10  | GLY  | 2              |
| 1   | A     | 72  | ASP  | 1              |
| 1   | B     | 72  | ASP  | 1              |
| 1   | A     | 15  | CYS  | 1              |
| 1   | B     | 15  | CYS  | 1              |
| 1   | A     | 69  | ARG  | 1              |
| 1   | A     | 73  | SER  | 1              |
| 1   | B     | 69  | ARG  | 1              |
| 1   | B     | 73  | SER  | 1              |
| 1   | A     | 20  | VAL  | 1              |
| 1   | B     | 20  | VAL  | 1              |
| 1   | A     | 78  | SER  | 1              |
| 1   | A     | 97  | ALA  | 1              |
| 1   | B     | 78  | SER  | 1              |
| 1   | B     | 97  | ALA  | 1              |
| 1   | A     | 11  | GLU  | 1              |
| 1   | B     | 11  | GLU  | 1              |
| 1   | A     | 67  | GLY  | 1              |
| 1   | B     | 67  | GLY  | 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     | 93/105 (89%)    | 91±1 (98±1%) | 2±1 (2±1%) | 48          | 91 |
| 1   | B     | 93/105 (89%)    | 91±1 (98±1%) | 2±1 (2±1%) | 46          | 90 |
| All | All   | 3720/4200 (89%) | 3643 (98%)   | 77 (2%)    | 46          | 90 |

All 41 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 30  | ASP  | 7              |
| 1   | B     | 30  | ASP  | 7              |
| 1   | A     | 82  | THR  | 5              |
| 1   | B     | 82  | THR  | 5              |
| 1   | B     | 41  | GLU  | 5              |
| 1   | A     | 41  | GLU  | 4              |
| 1   | A     | 64  | VAL  | 2              |
| 1   | B     | 64  | VAL  | 2              |
| 1   | A     | 112 | LEU  | 2              |
| 1   | B     | 112 | LEU  | 2              |
| 1   | A     | 11  | GLU  | 2              |
| 1   | B     | 11  | GLU  | 2              |
| 1   | A     | 96  | GLN  | 2              |
| 1   | B     | 96  | GLN  | 2              |
| 1   | A     | 88  | LYS  | 2              |
| 1   | A     | 43  | ASN  | 1              |
| 1   | A     | 74  | LYS  | 1              |
| 1   | B     | 43  | ASN  | 1              |
| 1   | B     | 74  | LYS  | 1              |
| 1   | A     | 95  | LYS  | 1              |
| 1   | B     | 95  | LYS  | 1              |
| 1   | A     | 25  | LYS  | 1              |
| 1   | B     | 25  | LYS  | 1              |
| 1   | A     | 16  | ASP  | 1              |
| 1   | B     | 16  | ASP  | 1              |
| 1   | A     | 32  | LYS  | 1              |
| 1   | B     | 32  | LYS  | 1              |
| 1   | A     | 50  | LYS  | 1              |
| 1   | A     | 52  | TYR  | 1              |
| 1   | B     | 50  | LYS  | 1              |
| 1   | B     | 52  | TYR  | 1              |
| 1   | A     | 62  | ASN  | 1              |
| 1   | B     | 62  | ASN  | 1              |
| 1   | A     | 83  | THR  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 83  | THR  | 1              |
| 1   | B     | 72  | ASP  | 1              |
| 1   | B     | 88  | LYS  | 1              |
| 1   | A     | 76  | TRP  | 1              |
| 1   | A     | 105 | ASP  | 1              |
| 1   | B     | 76  | TRP  | 1              |
| 1   | B     | 105 | ASP  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 39% for the well-defined parts and 38% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 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                  | 1208 |
| Number of shifts mapped to atoms        | 1208 |
| 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 108      | $0.18 \pm 0.08$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 104      | $0.11 \pm 0.23$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 105      | $0.55 \pm 0.59$                 | None needed (imprecise)    |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 39%, i.e. 1095 atoms were assigned a chemical shift out of a possible 2780. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 409/1056 (39%) | 212/430 (49%) | 100/420 (24%)   | 97/206 (47%)    |
| Sidechain | 649/1464 (44%) | 445/948 (47%) | 198/456 (43%)   | 6/60 (10%)      |

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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 | 37/260 (14%)    | 34/128 (27%)         | 0/118 (0%)            | 3/14 (21%)            |
| Overall  | 1095/2780 (39%) | 691/1506 (46%)       | 298/994 (30%)         | 106/280 (38%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 1207 atoms were assigned a chemical shift out of a possible 3164. 0 out of 32 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  | 444/1182 (38%)  | 231/480 (48%)        | 108/472 (23%)         | 105/230 (46%)         |
| Sidechain | 725/1670 (43%)  | 498/1082 (46%)       | 221/514 (43%)         | 6/74 (8%)             |
| Aromatic  | 38/312 (12%)    | 35/154 (23%)         | 0/136 (0%)            | 3/22 (14%)            |
| Overall   | 1207/3164 (38%) | 764/1716 (45%)       | 329/1122 (29%)        | 114/326 (35%)         |

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

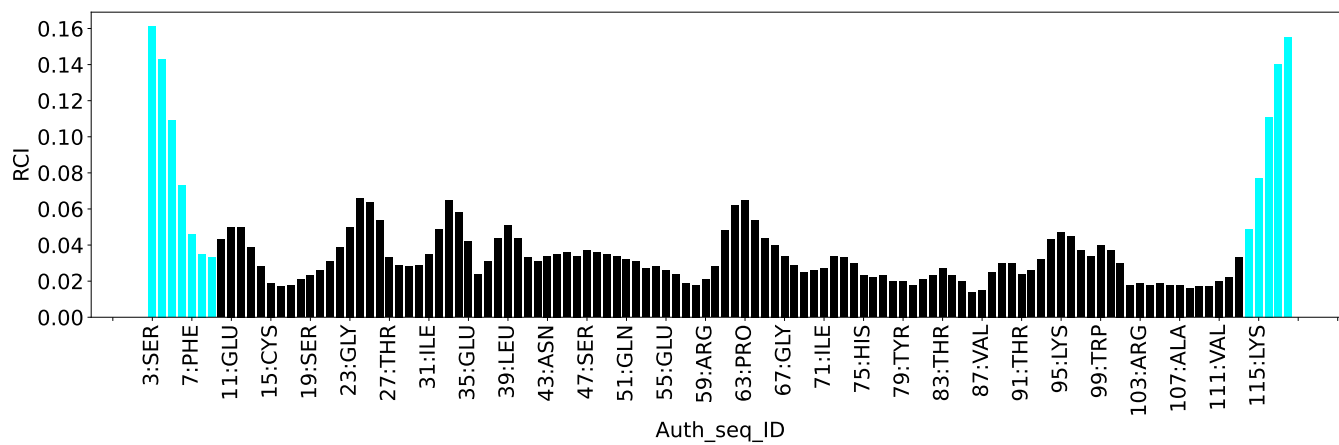
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 85  | THR  | HG1  | 6.42       | 0.08 – 2.19         | 25.0    |

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 3128  |
| Intra-residue ( $ i-j =0$ )                              | 1826  |
| Sequential ( $ i-j =1$ )                                 | 602   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 152   |
| Long range ( $ i-j \geq 5$ )                             | 492   |
| Inter-chain                                              | 56    |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 13.3  |
| Number of long range restraints per residue <sup>1</sup> | 2.1   |

<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)  | 54.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 122.8                                  | 0.5     |
| >0.5 (Large)     | 151.5                                  | 6.35    |

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

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

## 9 Distance violation analysis ⓘ

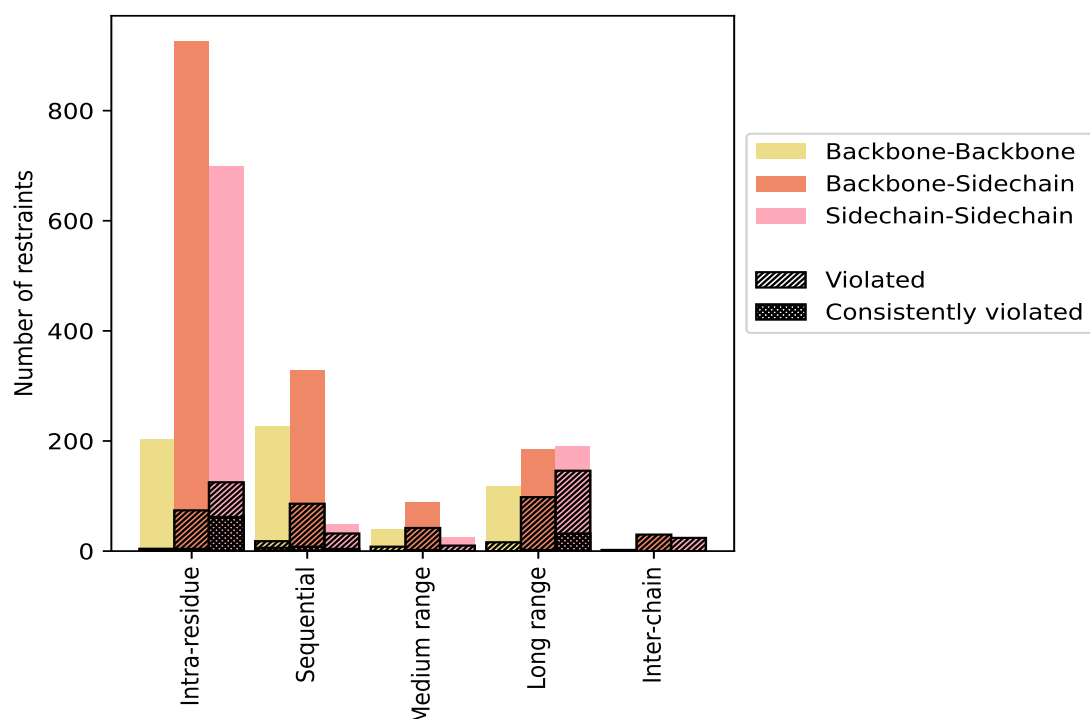
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>1826</b> | <b>58.4</b>    | <b>203</b>            | <b>11.1</b>    | <b>6.5</b>     | <b>70</b>                          | <b>3.8</b>     | <b>2.2</b>     |
| Backbone-Backbone                                                           | 202         | 6.5            | 4                     | 2.0            | 0.1            | 4                                  | 2.0            | 0.1            |
| Backbone-Sidechain                                                          | 926         | 29.6           | 74                    | 8.0            | 2.4            | 4                                  | 0.4            | 0.1            |
| Sidechain-Sidechain                                                         | 698         | 22.3           | 125                   | 17.9           | 4.0            | 62                                 | 8.9            | 2.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>602</b>  | <b>19.2</b>    | <b>136</b>            | <b>22.6</b>    | <b>4.3</b>     | <b>18</b>                          | <b>3.0</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 226         | 7.2            | 18                    | 8.0            | 0.6            | 6                                  | 2.7            | 0.2            |
| Backbone-Sidechain                                                          | 328         | 10.5           | 86                    | 26.2           | 2.7            | 8                                  | 2.4            | 0.3            |
| Sidechain-Sidechain                                                         | 48          | 1.5            | 32                    | 66.7           | 1.0            | 4                                  | 8.3            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>152</b>  | <b>4.9</b>     | <b>60</b>             | <b>39.5</b>    | <b>1.9</b>     | <b>2</b>                           | <b>1.3</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 40          | 1.3            | 8                     | 20.0           | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 88          | 2.8            | 42                    | 47.7           | 1.3            | 2                                  | 2.3            | 0.1            |
| Sidechain-Sidechain                                                         | 24          | 0.8            | 10                    | 41.7           | 0.3            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>492</b>  | <b>15.7</b>    | <b>260</b>            | <b>52.8</b>    | <b>8.3</b>     | <b>34</b>                          | <b>6.9</b>     | <b>1.1</b>     |
| Backbone-Backbone                                                           | 118         | 3.8            | 16                    | 13.6           | 0.5            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 184         | 5.9            | 98                    | 53.3           | 3.1            | 2                                  | 1.1            | 0.1            |
| Sidechain-Sidechain                                                         | 190         | 6.1            | 146                   | 76.8           | 4.7            | 32                                 | 16.8           | 1.0            |
| <b>Inter-chain</b>                                                          | <b>56</b>   | <b>1.8</b>     | <b>56</b>             | <b>100.0</b>   | <b>1.8</b>     | <b>2</b>                           | <b>3.6</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 2           | 0.1            | 2                     | 100.0          | 0.1            | 2                                  | 100.0          | 0.1            |
| Backbone-Sidechain                                                          | 30          | 1.0            | 30                    | 100.0          | 1.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 24          | 0.8            | 24                    | 100.0          | 0.8            | 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>3128</b> | <b>100.0</b>   | <b>715</b>            | <b>22.9</b>    | <b>22.9</b>    | <b>126</b>                         | <b>4.0</b>     | <b>4.0</b>     |
| Backbone-Backbone                                                           | 588         | 18.8           | 48                    | 8.2            | 1.5            | 12                                 | 2.0            | 0.4            |
| Backbone-Sidechain                                                          | 1556        | 49.7           | 330                   | 21.2           | 10.5           | 16                                 | 1.0            | 0.5            |
| Sidechain-Sidechain                                                         | 984         | 31.5           | 337                   | 34.2           | 10.8           | 98                                 | 10.0           | 3.1            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 117                  | 58              | 22              | 112             | 24              | 333   | 0.66     | 4.14    | 0.62                | 0.46       |
| 2        | 120                  | 62              | 10              | 96              | 30              | 318   | 0.64     | 3.57    | 0.58                | 0.45       |
| 3        | 108                  | 60              | 12              | 114             | 28              | 322   | 0.62     | 2.47    | 0.5                 | 0.46       |
| 4        | 114                  | 70              | 26              | 112             | 20              | 342   | 0.59     | 3.66    | 0.58                | 0.39       |
| 5        | 104                  | 62              | 18              | 124             | 32              | 340   | 0.76     | 3.67    | 0.68                | 0.5        |
| 6        | 117                  | 56              | 16              | 126             | 22              | 337   | 0.66     | 4.92    | 0.69                | 0.45       |
| 7        | 118                  | 74              | 20              | 122             | 29              | 363   | 0.73     | 3.41    | 0.68                | 0.48       |
| 8        | 114                  | 49              | 15              | 122             | 26              | 326   | 0.82     | 5.13    | 0.85                | 0.56       |
| 9        | 118                  | 62              | 14              | 122             | 28              | 344   | 0.72     | 5.57    | 0.76                | 0.49       |
| 10       | 110                  | 64              | 20              | 113             | 28              | 335   | 0.72     | 6.35    | 0.75                | 0.48       |

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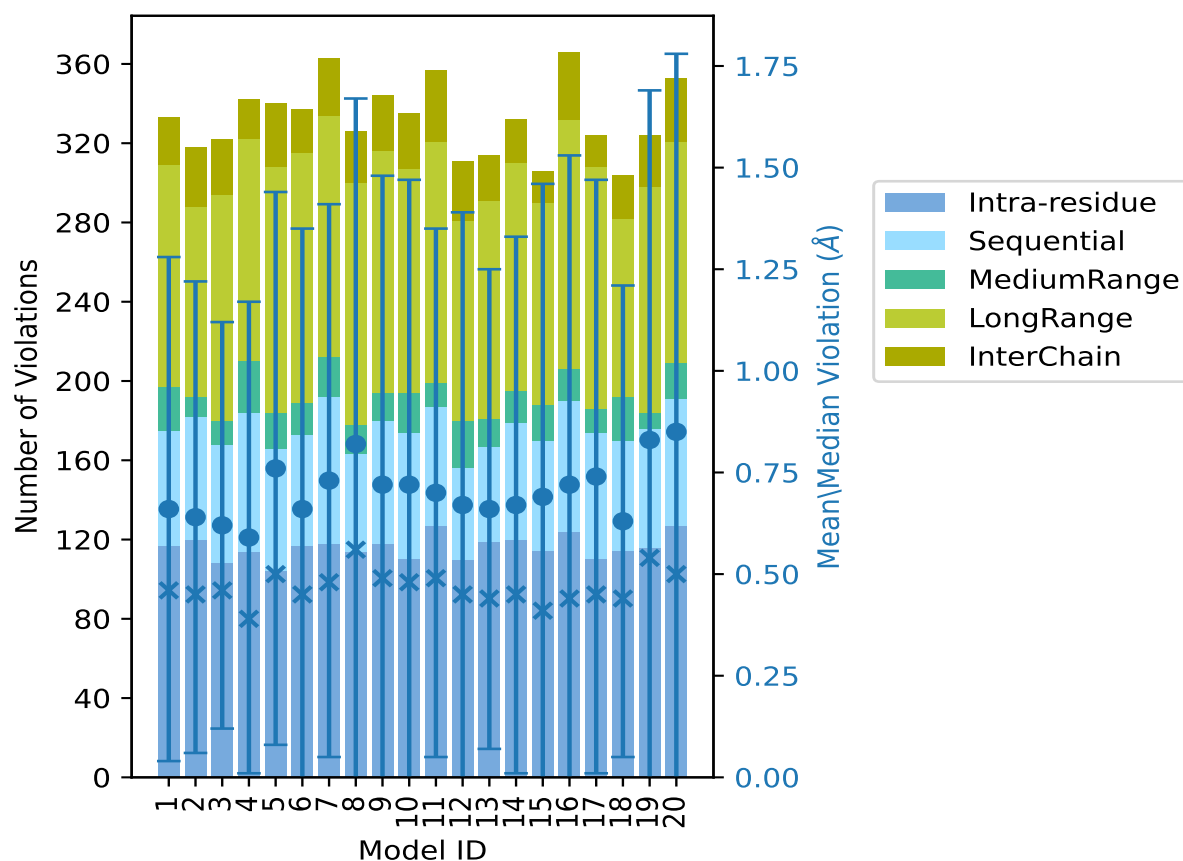
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 127                  | 60              | 12              | 122             | 36              | 357   | 0.7      | 3.74    | 0.65                | 0.49       |
| 12       | 110                  | 46              | 24              | 101             | 30              | 311   | 0.67     | 5.48    | 0.72                | 0.45       |
| 13       | 119                  | 48              | 14              | 110             | 23              | 314   | 0.66     | 3.45    | 0.59                | 0.44       |
| 14       | 120                  | 59              | 16              | 115             | 22              | 332   | 0.67     | 3.39    | 0.66                | 0.45       |
| 15       | 114                  | 56              | 18              | 102             | 16              | 306   | 0.69     | 5.25    | 0.77                | 0.41       |
| 16       | 124                  | 66              | 16              | 126             | 34              | 366   | 0.72     | 5.53    | 0.81                | 0.44       |
| 17       | 110                  | 64              | 12              | 122             | 16              | 324   | 0.74     | 3.78    | 0.73                | 0.45       |
| 18       | 114                  | 56              | 22              | 90              | 22              | 304   | 0.63     | 3.28    | 0.58                | 0.44       |
| 19       | 116                  | 60              | 8               | 114             | 26              | 324   | 0.83     | 4.81    | 0.86                | 0.54       |
| 20       | 127                  | 64              | 18              | 112             | 32              | 353   | 0.85     | 4.95    | 0.93                | 0.5        |

<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

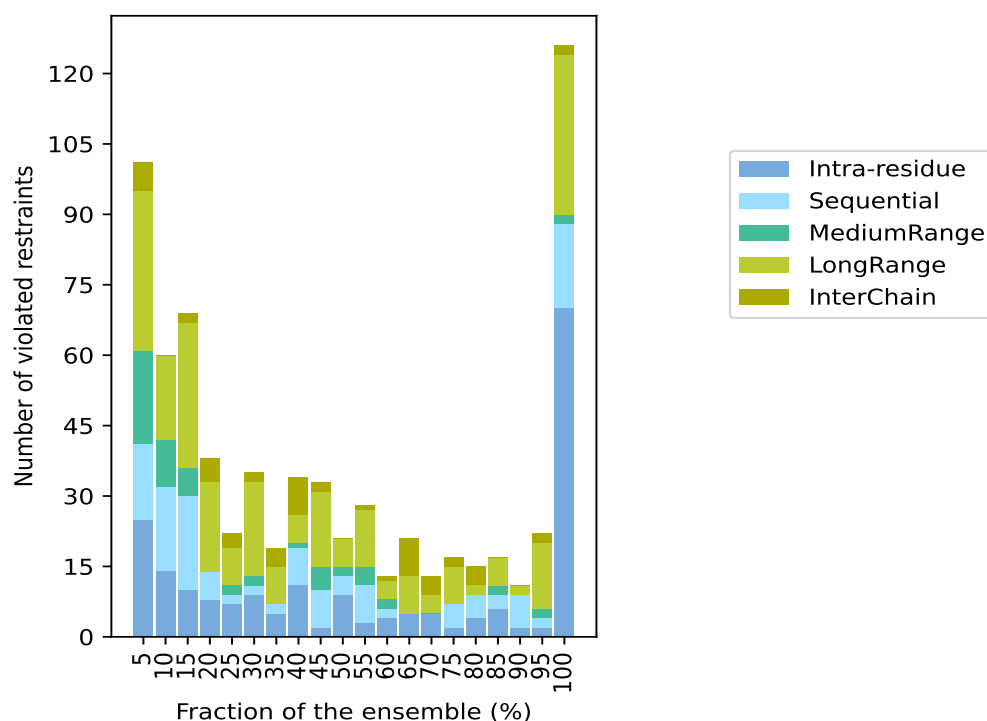
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2413(IR:1623, SQ:466, MR:92, LR:232, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 25                            | 16              | 20              | 34              | 6               | 101   | 1                        | 5.0   |
| 14                            | 18              | 10              | 18              | 0               | 60    | 2                        | 10.0  |
| 10                            | 20              | 6               | 31              | 2               | 69    | 3                        | 15.0  |
| 8                             | 6               | 0               | 19              | 5               | 38    | 4                        | 20.0  |
| 7                             | 2               | 2               | 8               | 3               | 22    | 5                        | 25.0  |
| 9                             | 2               | 2               | 20              | 2               | 35    | 6                        | 30.0  |
| 5                             | 2               | 0               | 8               | 4               | 19    | 7                        | 35.0  |
| 11                            | 8               | 1               | 6               | 8               | 34    | 8                        | 40.0  |
| 2                             | 8               | 5               | 16              | 2               | 33    | 9                        | 45.0  |
| 9                             | 4               | 2               | 6               | 0               | 21    | 10                       | 50.0  |
| 3                             | 8               | 4               | 12              | 1               | 28    | 11                       | 55.0  |
| 4                             | 2               | 2               | 4               | 1               | 13    | 12                       | 60.0  |
| 5                             | 0               | 0               | 8               | 8               | 21    | 13                       | 65.0  |
| 5                             | 0               | 0               | 4               | 4               | 13    | 14                       | 70.0  |
| 2                             | 5               | 0               | 8               | 2               | 17    | 15                       | 75.0  |
| 4                             | 5               | 0               | 2               | 4               | 15    | 16                       | 80.0  |
| 6                             | 3               | 2               | 6               | 0               | 17    | 17                       | 85.0  |
| 2                             | 7               | 0               | 2               | 0               | 11    | 18                       | 90.0  |
| 2                             | 2               | 2               | 14              | 2               | 22    | 19                       | 95.0  |
| 70                            | 18              | 2               | 34              | 2               | 126   | 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

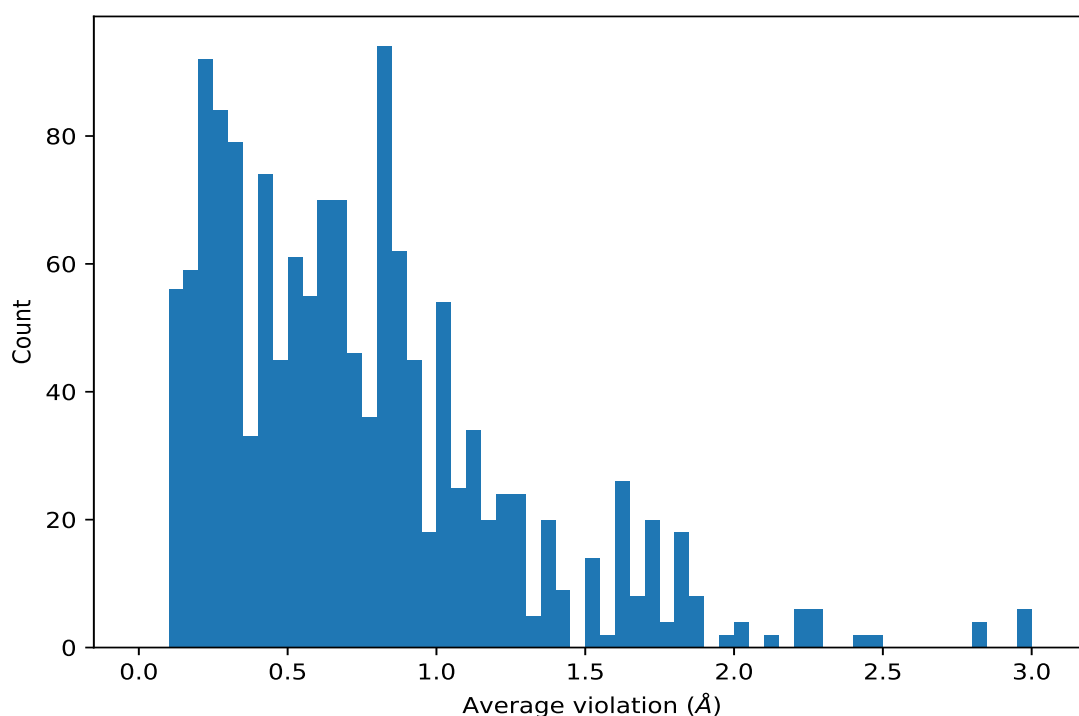
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1389) | 1:57:A:LYS:HE2 | 1:18:A:VAL:HG13 | 20                  | 2.97     | 1.31                | 2.98       |
| (1,1389) | 1:57:A:LYS:HE2 | 1:18:A:VAL:HG12 | 20                  | 2.97     | 1.31                | 2.98       |
| (1,1389) | 1:57:A:LYS:HE2 | 1:18:A:VAL:HG11 | 20                  | 2.97     | 1.31                | 2.98       |
| (1,1390) | 1:57:B:LYS:HE2 | 1:18:B:VAL:HG13 | 20                  | 2.97     | 1.31                | 2.96       |
| (1,1390) | 1:57:B:LYS:HE2 | 1:18:B:VAL:HG12 | 20                  | 2.97     | 1.31                | 2.96       |
| (1,1390) | 1:57:B:LYS:HE2 | 1:18:B:VAL:HG11 | 20                  | 2.97     | 1.31                | 2.96       |
| (1,886)  | 1:22:B:VAL:HB  | 1:53:B:PHE:HB3  | 20                  | 1.99     | 0.47                | 1.84       |
| (1,885)  | 1:22:A:VAL:HB  | 1:53:A:PHE:HB3  | 20                  | 1.99     | 0.47                | 1.85       |
| (1,3084) | 1:13:B:SER:H   | 1:111:A:VAL:HA  | 20                  | 1.87     | 1.32                | 1.34       |
| (1,3083) | 1:13:A:SER:H   | 1:111:B:VAL:HA  | 20                  | 1.87     | 1.32                | 1.34       |
| (1,225)  | 1:63:A:PRO:HB3 | 1:64:A:VAL:HG22 | 20                  | 1.87     | 0.72                | 1.59       |
| (1,225)  | 1:63:A:PRO:HB3 | 1:64:A:VAL:HG23 | 20                  | 1.87     | 0.72                | 1.59       |
| (1,225)  | 1:63:A:PRO:HB3 | 1:64:A:VAL:HG21 | 20                  | 1.87     | 0.72                | 1.59       |
| (1,226)  | 1:63:B:PRO:HB3 | 1:64:B:VAL:HG22 | 20                  | 1.87     | 0.72                | 1.59       |
| (1,226)  | 1:63:B:PRO:HB3 | 1:64:B:VAL:HG23 | 20                  | 1.87     | 0.72                | 1.59       |
| (1,226)  | 1:63:B:PRO:HB3 | 1:64:B:VAL:HG21 | 20                  | 1.87     | 0.72                | 1.59       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,549)  | 1:92:A:MET:HE3   | 1:97:A:ALA:HB3  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,549)  | 1:92:A:MET:HE1   | 1:97:A:ALA:HB3  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB2  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB3  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB1  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,549)  | 1:92:A:MET:HE1   | 1:97:A:ALA:HB2  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,549)  | 1:92:A:MET:HE1   | 1:97:A:ALA:HB1  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,549)  | 1:92:A:MET:HE3   | 1:97:A:ALA:HB1  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE3   | 1:97:B:ALA:HB3  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE1   | 1:97:B:ALA:HB3  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB2  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB3  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB1  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE1   | 1:97:B:ALA:HB2  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE1   | 1:97:B:ALA:HB1  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,550)  | 1:92:B:MET:HE3   | 1:97:B:ALA:HB1  | 20                  | 1.72     | 1.13                | 1.48       |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3  | 20                  | 1.6      | 0.51                | 1.42       |
| (1,95)   | 1:22:A:VAL:HG13  | 1:53:A:PHE:HB3  | 20                  | 1.6      | 0.51                | 1.42       |
| (1,95)   | 1:22:A:VAL:HG12  | 1:53:A:PHE:HB3  | 20                  | 1.6      | 0.51                | 1.42       |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3  | 20                  | 1.6      | 0.51                | 1.42       |
| (1,96)   | 1:22:B:VAL:HG13  | 1:53:B:PHE:HB3  | 20                  | 1.6      | 0.51                | 1.42       |
| (1,96)   | 1:22:B:VAL:HG12  | 1:53:B:PHE:HB3  | 20                  | 1.6      | 0.51                | 1.42       |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA   | 20                  | 1.35     | 0.33                | 1.34       |
| (1,179)  | 1:109:A:VAL:HG21 | 1:81:A:THR:HA   | 20                  | 1.35     | 0.33                | 1.34       |
| (1,179)  | 1:109:A:VAL:HG22 | 1:81:A:THR:HA   | 20                  | 1.35     | 0.33                | 1.34       |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA   | 20                  | 1.35     | 0.33                | 1.34       |
| (1,180)  | 1:109:B:VAL:HG21 | 1:81:B:THR:HA   | 20                  | 1.35     | 0.33                | 1.34       |
| (1,180)  | 1:109:B:VAL:HG22 | 1:81:B:THR:HA   | 20                  | 1.35     | 0.33                | 1.34       |
| (1,922)  | 1:116:B:ALA:HB2  | 1:115:B:LYS:HA  | 20                  | 1.19     | 0.41                | 1.04       |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA  | 20                  | 1.19     | 0.41                | 1.04       |
| (1,922)  | 1:116:B:ALA:HB1  | 1:115:B:LYS:HA  | 20                  | 1.19     | 0.41                | 1.04       |
| (1,921)  | 1:116:A:ALA:HB2  | 1:115:A:LYS:HA  | 20                  | 1.19     | 0.41                | 1.04       |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA  | 20                  | 1.19     | 0.41                | 1.04       |
| (1,921)  | 1:116:A:ALA:HB1  | 1:115:A:LYS:HA  | 20                  | 1.19     | 0.41                | 1.04       |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2  | 20                  | 1.14     | 0.35                | 1.21       |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2  | 20                  | 1.14     | 0.36                | 1.21       |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG23 | 20                  | 1.12     | 0.56                | 0.93       |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG22 | 20                  | 1.12     | 0.56                | 0.93       |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21 | 20                  | 1.12     | 0.56                | 0.93       |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG23 | 20                  | 1.12     | 0.56                | 0.93       |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG22 | 20                  | 1.12     | 0.56                | 0.93       |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21 | 20                  | 1.12     | 0.56                | 0.93       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1204) | 1:37:B:MET:HE2  | 1:26:B:THR:HG21 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1204) | 1:37:B:MET:HE1  | 1:26:B:THR:HG23 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1204) | 1:37:B:MET:HE1  | 1:26:B:THR:HG21 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1204) | 1:37:B:MET:HE3  | 1:26:B:THR:HG23 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1204) | 1:37:B:MET:HE3  | 1:26:B:THR:HG22 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1204) | 1:37:B:MET:HE3  | 1:26:B:THR:HG21 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1204) | 1:37:B:MET:HE1  | 1:26:B:THR:HG22 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1204) | 1:37:B:MET:HE2  | 1:26:B:THR:HG23 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE2  | 1:26:A:THR:HG21 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE1  | 1:26:A:THR:HG23 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE1  | 1:26:A:THR:HG21 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE3  | 1:26:A:THR:HG23 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE3  | 1:26:A:THR:HG22 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE3  | 1:26:A:THR:HG21 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE1  | 1:26:A:THR:HG22 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1203) | 1:37:A:MET:HE2  | 1:26:A:THR:HG23 | 20                  | 1.09     | 1.1                 | 0.42       |
| (1,1319) | 1:34:A:LYS:HD2  | 1:34:A:LYS:HB3  | 20                  | 1.04     | 0.09                | 1.04       |
| (1,1320) | 1:34:B:LYS:HD2  | 1:34:B:LYS:HB3  | 20                  | 1.04     | 0.09                | 1.04       |
| (1,936)  | 1:98:B:ALA:HA   | 1:97:B:ALA:HB1  | 20                  | 0.93     | 0.12                | 0.89       |
| (1,936)  | 1:98:B:ALA:HA   | 1:97:B:ALA:HB3  | 20                  | 0.93     | 0.12                | 0.89       |
| (1,936)  | 1:98:B:ALA:HA   | 1:97:B:ALA:HB2  | 20                  | 0.93     | 0.12                | 0.89       |
| (1,935)  | 1:98:A:ALA:HA   | 1:97:A:ALA:HB1  | 20                  | 0.93     | 0.12                | 0.88       |
| (1,935)  | 1:98:A:ALA:HA   | 1:97:A:ALA:HB3  | 20                  | 0.93     | 0.12                | 0.88       |
| (1,935)  | 1:98:A:ALA:HA   | 1:97:A:ALA:HB2  | 20                  | 0.93     | 0.12                | 0.88       |
| (1,1206) | 1:27:B:THR:HA   | 1:26:B:THR:HG21 | 20                  | 0.91     | 0.14                | 0.92       |
| (1,1206) | 1:27:B:THR:HA   | 1:26:B:THR:HG23 | 20                  | 0.91     | 0.14                | 0.92       |
| (1,1206) | 1:27:B:THR:HA   | 1:26:B:THR:HG22 | 20                  | 0.91     | 0.14                | 0.92       |
| (1,1205) | 1:27:A:THR:HA   | 1:26:A:THR:HG21 | 20                  | 0.9      | 0.13                | 0.92       |
| (1,1205) | 1:27:A:THR:HA   | 1:26:A:THR:HG23 | 20                  | 0.9      | 0.13                | 0.92       |
| (1,1205) | 1:27:A:THR:HA   | 1:26:A:THR:HG22 | 20                  | 0.9      | 0.13                | 0.92       |
| (1,51)   | 1:42:A:VAL:HG22 | 1:42:A:VAL:HG11 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,51)   | 1:42:A:VAL:HG23 | 1:42:A:VAL:HG13 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,51)   | 1:42:A:VAL:HG21 | 1:42:A:VAL:HG11 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,51)   | 1:42:A:VAL:HG23 | 1:42:A:VAL:HG12 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,51)   | 1:42:A:VAL:HG21 | 1:42:A:VAL:HG13 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,51)   | 1:42:A:VAL:HG22 | 1:42:A:VAL:HG13 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,51)   | 1:42:A:VAL:HG23 | 1:42:A:VAL:HG11 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,51)   | 1:42:A:VAL:HG22 | 1:42:A:VAL:HG12 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,52)   | 1:42:B:VAL:HG22 | 1:42:B:VAL:HG11 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,52)   | 1:42:B:VAL:HG23 | 1:42:B:VAL:HG13 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,52)   | 1:42:B:VAL:HG21 | 1:42:B:VAL:HG11 | 20                  | 0.89     | 0.02                | 0.89       |
| (1,52)   | 1:42:B:VAL:HG23 | 1:42:B:VAL:HG12 | 20                  | 0.89     | 0.02                | 0.89       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,52)  | 1:42:B:VAL:HG21  | 1:42:B:VAL:HG13  | 20                  | 0.89     | 0.02                | 0.89       |
| (1,52)  | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG13  | 20                  | 0.89     | 0.02                | 0.89       |
| (1,52)  | 1:42:B:VAL:HG23  | 1:42:B:VAL:HG11  | 20                  | 0.89     | 0.02                | 0.89       |
| (1,52)  | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG12  | 20                  | 0.89     | 0.02                | 0.89       |
| (1,427) | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG21  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,427) | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG22  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,427) | 1:87:A:VAL:HG13  | 1:87:A:VAL:HG23  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,427) | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG23  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,427) | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG22  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,427) | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG23  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,427) | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG21  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,428) | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG21  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,428) | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG22  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,428) | 1:87:B:VAL:HG13  | 1:87:B:VAL:HG23  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,428) | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG23  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,428) | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG22  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,428) | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG23  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,428) | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG21  | 20                  | 0.87     | 0.02                | 0.88       |
| (1,288) | 1:106:B:THR:HG22 | 1:85:B:THR:HG22  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,288) | 1:106:B:THR:HG23 | 1:85:B:THR:HG23  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,288) | 1:106:B:THR:HG21 | 1:85:B:THR:HG21  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,288) | 1:106:B:THR:HG21 | 1:85:B:THR:HG22  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,288) | 1:106:B:THR:HG23 | 1:85:B:THR:HG21  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,288) | 1:106:B:THR:HG22 | 1:85:B:THR:HG21  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,288) | 1:106:B:THR:HG21 | 1:85:B:THR:HG23  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,288) | 1:106:B:THR:HG22 | 1:85:B:THR:HG23  | 20                  | 0.84     | 0.24                | 0.84       |
| (1,287) | 1:106:A:THR:HG22 | 1:85:A:THR:HG22  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,287) | 1:106:A:THR:HG23 | 1:85:A:THR:HG23  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,287) | 1:106:A:THR:HG21 | 1:85:A:THR:HG21  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,287) | 1:106:A:THR:HG21 | 1:85:A:THR:HG22  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,287) | 1:106:A:THR:HG23 | 1:85:A:THR:HG21  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,287) | 1:106:A:THR:HG22 | 1:85:A:THR:HG21  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,287) | 1:106:A:THR:HG21 | 1:85:A:THR:HG23  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,287) | 1:106:A:THR:HG22 | 1:85:A:THR:HG23  | 20                  | 0.84     | 0.23                | 0.84       |
| (1,761) | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG13 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,761) | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG11 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,761) | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG12 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,761) | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG12 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,761) | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG12 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,761) | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG11 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,761) | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG11 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,761) | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG13 | 20                  | 0.82     | 0.03                | 0.83       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG13 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG13 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG11 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG12 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG12 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG12 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG11 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG11 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG13 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG13 | 20                  | 0.82     | 0.03                | 0.83       |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB3   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1430) | 1:102:B:ILE:HD11 | 1:28:B:ALA:HB3   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB3   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB2   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB2   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1430) | 1:102:B:ILE:HD11 | 1:28:B:ALA:HB1   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB1   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB1   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB3   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD11 | 1:28:A:ALA:HB3   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB3   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB2   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB2   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD11 | 1:28:A:ALA:HB1   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB1   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB1   | 20                  | 0.77     | 0.14                | 0.74       |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG13 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG13 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,923)  | 1:81:A:THR:HG22  | 1:111:A:VAL:HG11 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG11 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG11 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG12 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,923)  | 1:81:A:THR:HG22  | 1:111:A:VAL:HG12 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG12 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG13 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG13 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG22  | 1:111:B:VAL:HG11 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG11 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG11 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG12 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG22  | 1:111:B:VAL:HG12 | 20                  | 0.7      | 0.2                 | 0.7        |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG12 | 20                  | 0.7      | 0.2                 | 0.7        |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1436) | 1:38:B:VAL:HG21  | 1:28:B:ALA:HB3  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB3  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB2  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB3  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB2  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB1  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1436) | 1:38:B:VAL:HG21  | 1:28:B:ALA:HB1  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB1  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG21  | 1:28:A:ALA:HB3  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB3  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB2  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB3  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB2  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB1  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG21  | 1:28:A:ALA:HB1  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB1  | 20                  | 0.69     | 0.26                | 0.62       |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG21 | 20                  | 0.69     | 0.03                | 0.69       |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG22 | 20                  | 0.69     | 0.03                | 0.69       |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG23 | 20                  | 0.69     | 0.03                | 0.69       |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG23 | 20                  | 0.69     | 0.03                | 0.69       |
| (1,771)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HG22 | 20                  | 0.69     | 0.03                | 0.69       |
| (1,771)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HG23 | 20                  | 0.69     | 0.03                | 0.69       |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG21 | 20                  | 0.69     | 0.03                | 0.69       |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG21 | 20                  | 0.68     | 0.03                | 0.69       |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG22 | 20                  | 0.68     | 0.03                | 0.69       |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG23 | 20                  | 0.68     | 0.03                | 0.69       |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG23 | 20                  | 0.68     | 0.03                | 0.69       |
| (1,772)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HG22 | 20                  | 0.68     | 0.03                | 0.69       |
| (1,772)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HG23 | 20                  | 0.68     | 0.03                | 0.69       |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG21 | 20                  | 0.68     | 0.03                | 0.69       |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG13 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG11 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG11 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG11 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG12 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG12 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG13 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG12 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG13 | 20                  | 0.68     | 0.24                | 0.62       |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG13 | 20                  | 0.68     | 0.24                | 0.63       |
| (1,390)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG11 | 20                  | 0.68     | 0.24                | 0.63       |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG11 | 20                  | 0.68     | 0.24                | 0.63       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,390) | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG11  | 20                  | 0.68     | 0.24                | 0.63       |
| (1,390) | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG12  | 20                  | 0.68     | 0.24                | 0.63       |
| (1,390) | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG12  | 20                  | 0.68     | 0.24                | 0.63       |
| (1,390) | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG13  | 20                  | 0.68     | 0.24                | 0.63       |
| (1,390) | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG12  | 20                  | 0.68     | 0.24                | 0.63       |
| (1,390) | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG13  | 20                  | 0.68     | 0.24                | 0.63       |
| (1,765) | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG21  | 20                  | 0.66     | 0.13                | 0.68       |
| (1,765) | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22  | 20                  | 0.66     | 0.13                | 0.68       |
| (1,765) | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23  | 20                  | 0.66     | 0.13                | 0.68       |
| (1,766) | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG21  | 20                  | 0.66     | 0.13                | 0.68       |
| (1,766) | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22  | 20                  | 0.66     | 0.13                | 0.68       |
| (1,766) | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23  | 20                  | 0.66     | 0.13                | 0.68       |
| (1,542) | 1:92:B:MET:HE2   | 1:39:B:LEU:HD11  | 20                  | 0.64     | 0.37                | 0.59       |
| (1,542) | 1:92:B:MET:HE3   | 1:39:B:LEU:HD12  | 20                  | 0.64     | 0.37                | 0.59       |
| (1,542) | 1:92:B:MET:HE1   | 1:39:B:LEU:HD11  | 20                  | 0.64     | 0.37                | 0.59       |
| (1,542) | 1:92:B:MET:HE1   | 1:39:B:LEU:HD12  | 20                  | 0.64     | 0.37                | 0.59       |
| (1,542) | 1:92:B:MET:HE3   | 1:39:B:LEU:HD11  | 20                  | 0.64     | 0.37                | 0.59       |
| (1,542) | 1:92:B:MET:HE2   | 1:39:B:LEU:HD13  | 20                  | 0.64     | 0.37                | 0.59       |
| (1,542) | 1:92:B:MET:HE2   | 1:39:B:LEU:HD12  | 20                  | 0.64     | 0.37                | 0.59       |
| (1,541) | 1:92:A:MET:HE2   | 1:39:A:LEU:HD11  | 20                  | 0.64     | 0.37                | 0.58       |
| (1,541) | 1:92:A:MET:HE3   | 1:39:A:LEU:HD12  | 20                  | 0.64     | 0.37                | 0.58       |
| (1,541) | 1:92:A:MET:HE1   | 1:39:A:LEU:HD11  | 20                  | 0.64     | 0.37                | 0.58       |
| (1,541) | 1:92:A:MET:HE1   | 1:39:A:LEU:HD12  | 20                  | 0.64     | 0.37                | 0.58       |
| (1,541) | 1:92:A:MET:HE3   | 1:39:A:LEU:HD11  | 20                  | 0.64     | 0.37                | 0.58       |
| (1,541) | 1:92:A:MET:HE2   | 1:39:A:LEU:HD13  | 20                  | 0.64     | 0.37                | 0.58       |
| (1,541) | 1:92:A:MET:HE2   | 1:39:A:LEU:HD12  | 20                  | 0.64     | 0.37                | 0.58       |
| (1,10)  | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG11 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,10)  | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG13 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,10)  | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG11 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,10)  | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG12 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,10)  | 1:111:B:VAL:HG23 | 1:111:B:VAL:HG11 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,10)  | 1:111:B:VAL:HG23 | 1:111:B:VAL:HG13 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,10)  | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG12 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,10)  | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG13 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG11 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG13 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG11 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG12 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG23 | 1:111:A:VAL:HG11 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG23 | 1:111:A:VAL:HG13 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG12 | 20                  | 0.63     | 0.02                | 0.63       |
| (1,9)   | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG13 | 20                  | 0.63     | 0.02                | 0.63       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG22 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD12 | 1:87:B:VAL:HG22 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG23 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG23 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG21 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD12 | 1:87:B:VAL:HG21 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD12 | 1:87:B:VAL:HG23 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG22 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG21 | 20                  | 0.58     | 0.21                | 0.54       |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG22 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD12 | 1:87:A:VAL:HG22 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG23 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG23 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG21 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD12 | 1:87:A:VAL:HG21 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD12 | 1:87:A:VAL:HG23 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG22 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG21 | 20                  | 0.58     | 0.21                | 0.53       |
| (1,1168) | 1:92:B:MET:HE3   | 1:92:B:MET:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (1,1168) | 1:92:B:MET:HE2   | 1:92:B:MET:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (1,1167) | 1:92:A:MET:HE3   | 1:92:A:MET:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG21 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG22 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG22 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG23 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG23 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG23 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG22 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG21 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG21 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG21 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG22 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG22 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG23 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG23 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG23 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG22 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG21 | 20                  | 0.51     | 0.06                | 0.5        |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG21 | 20                  | 0.51     | 0.06                | 0.5        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 20                  | 0.5      | 0.23                | 0.39       |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 20                  | 0.5      | 0.23                | 0.39       |
| (1,1219) | 1:20:A:VAL:HG22  | 1:20:A:VAL:HB    | 20                  | 0.5      | 0.01                | 0.5        |
| (1,1219) | 1:20:A:VAL:HG21  | 1:20:A:VAL:HB    | 20                  | 0.5      | 0.01                | 0.5        |
| (1,1219) | 1:20:A:VAL:HG23  | 1:20:A:VAL:HB    | 20                  | 0.5      | 0.01                | 0.5        |
| (1,1220) | 1:20:B:VAL:HG22  | 1:20:B:VAL:HB    | 20                  | 0.5      | 0.01                | 0.5        |
| (1,1220) | 1:20:B:VAL:HG21  | 1:20:B:VAL:HB    | 20                  | 0.5      | 0.01                | 0.5        |
| (1,1220) | 1:20:B:VAL:HG23  | 1:20:B:VAL:HB    | 20                  | 0.5      | 0.01                | 0.5        |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 20                  | 0.49     | 0.01                | 0.5        |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB    | 20                  | 0.49     | 0.01                | 0.5        |
| (1,349)  | 1:48:A:VAL:HG11  | 1:48:A:VAL:HB    | 20                  | 0.49     | 0.01                | 0.5        |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB    | 20                  | 0.49     | 0.01                | 0.49       |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB    | 20                  | 0.49     | 0.01                | 0.49       |
| (1,350)  | 1:48:B:VAL:HG11  | 1:48:B:VAL:HB    | 20                  | 0.49     | 0.01                | 0.49       |
| (1,1017) | 1:18:A:VAL:HG22  | 1:18:A:VAL:HB    | 20                  | 0.48     | 0.0                 | 0.48       |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 20                  | 0.48     | 0.0                 | 0.48       |
| (1,1017) | 1:18:A:VAL:HG23  | 1:18:A:VAL:HB    | 20                  | 0.48     | 0.0                 | 0.48       |
| (1,1018) | 1:18:B:VAL:HG22  | 1:18:B:VAL:HB    | 20                  | 0.48     | 0.0                 | 0.48       |
| (1,1018) | 1:18:B:VAL:HG21  | 1:18:B:VAL:HB    | 20                  | 0.48     | 0.0                 | 0.48       |
| (1,1018) | 1:18:B:VAL:HG23  | 1:18:B:VAL:HB    | 20                  | 0.48     | 0.0                 | 0.48       |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 20                  | 0.46     | 0.12                | 0.47       |
| (1,596)  | 1:107:B:ALA:HB2  | 1:106:B:THR:HA   | 20                  | 0.46     | 0.12                | 0.47       |
| (1,596)  | 1:107:B:ALA:HB3  | 1:106:B:THR:HA   | 20                  | 0.46     | 0.12                | 0.47       |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 20                  | 0.46     | 0.13                | 0.47       |
| (1,595)  | 1:107:A:ALA:HB2  | 1:106:A:THR:HA   | 20                  | 0.46     | 0.13                | 0.47       |
| (1,595)  | 1:107:A:ALA:HB3  | 1:106:A:THR:HA   | 20                  | 0.46     | 0.13                | 0.47       |
| (1,383)  | 1:104:A:ILE:HG22 | 1:104:A:ILE:HD13 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD12 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD12 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,383)  | 1:104:A:ILE:HG22 | 1:104:A:ILE:HD11 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD13 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,383)  | 1:104:A:ILE:HG22 | 1:104:A:ILE:HD12 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD13 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,384)  | 1:104:B:ILE:HG22 | 1:104:B:ILE:HD13 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD12 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD12 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,384)  | 1:104:B:ILE:HG22 | 1:104:B:ILE:HD11 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD13 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,384)  | 1:104:B:ILE:HG22 | 1:104:B:ILE:HD12 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD13 | 20                  | 0.43     | 0.03                | 0.44       |
| (1,1233) | 1:47:A:SER:HB2   | 1:47:A:SER:HB3   | 20                  | 0.4      | 0.0                 | 0.4        |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 20                  | 0.4      | 0.0                 | 0.4        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 20                  | 0.4      | 0.05                | 0.42       |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 20                  | 0.4      | 0.05                | 0.42       |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 20                  | 0.35     | 0.3                 | 0.28       |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 20                  | 0.35     | 0.3                 | 0.26       |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG21  | 20                  | 0.33     | 0.02                | 0.33       |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 20                  | 0.33     | 0.02                | 0.33       |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG22  | 20                  | 0.33     | 0.02                | 0.33       |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG21  | 20                  | 0.33     | 0.03                | 0.33       |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 20                  | 0.33     | 0.03                | 0.33       |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG22  | 20                  | 0.33     | 0.03                | 0.33       |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG13 | 20                  | 0.32     | 0.01                | 0.32       |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 20                  | 0.32     | 0.01                | 0.32       |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG12 | 20                  | 0.32     | 0.01                | 0.32       |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 20                  | 0.32     | 0.01                | 0.32       |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 20                  | 0.32     | 0.01                | 0.32       |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG13 | 20                  | 0.32     | 0.01                | 0.32       |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 20                  | 0.32     | 0.03                | 0.32       |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB3   | 20                  | 0.32     | 0.03                | 0.32       |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB2   | 20                  | 0.32     | 0.03                | 0.32       |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 20                  | 0.32     | 0.03                | 0.32       |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB3   | 20                  | 0.32     | 0.03                | 0.32       |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB2   | 20                  | 0.32     | 0.03                | 0.32       |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 20                  | 0.31     | 0.0                 | 0.31       |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG11  | 20                  | 0.31     | 0.0                 | 0.31       |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 20                  | 0.31     | 0.0                 | 0.31       |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 20                  | 0.31     | 0.0                 | 0.31       |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG11  | 20                  | 0.31     | 0.0                 | 0.31       |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 20                  | 0.31     | 0.0                 | 0.31       |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD12 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD12 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 20                  | 0.29     | 0.21                | 0.21       |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 20                  | 0.29     | 0.21                | 0.21       |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 20                  | 0.28     | 0.01                | 0.28       |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 20                  | 0.28     | 0.01                | 0.28       |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG21  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG21  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1353) | 1:104:A:ILE:HD11 | 1:87:A:VAL:HG21  | 20                  | 0.26     | 0.06                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG23  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG23  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG22  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG21  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG21  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1354) | 1:104:B:ILE:HD11 | 1:87:B:VAL:HG21  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG23  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG23  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG22  | 20                  | 0.26     | 0.06                | 0.24       |
| (1,701)  | 1:37:A:MET:HB2   | 1:37:A:MET:HB3   | 20                  | 0.25     | 0.0                 | 0.25       |
| (1,702)  | 1:37:B:MET:HB2   | 1:37:B:MET:HB3   | 20                  | 0.25     | 0.0                 | 0.25       |
| (1,151)  | 1:100:A:ARG:HG3  | 1:100:A:ARG:HG2  | 20                  | 0.24     | 0.0                 | 0.24       |
| (1,152)  | 1:100:B:ARG:HG3  | 1:100:B:ARG:HG2  | 20                  | 0.24     | 0.0                 | 0.24       |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23  | 20                  | 0.23     | 0.02                | 0.24       |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG22  | 20                  | 0.23     | 0.02                | 0.24       |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG21  | 20                  | 0.23     | 0.02                | 0.24       |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23  | 20                  | 0.23     | 0.02                | 0.24       |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG22  | 20                  | 0.23     | 0.02                | 0.24       |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG21  | 20                  | 0.23     | 0.02                | 0.24       |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 20                  | 0.23     | 0.0                 | 0.23       |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 20                  | 0.23     | 0.0                 | 0.23       |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 20                  | 0.23     | 0.07                | 0.21       |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 20                  | 0.22     | 0.07                | 0.2        |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 20                  | 0.22     | 0.01                | 0.22       |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 20                  | 0.22     | 0.01                | 0.22       |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG12  | 20                  | 0.22     | 0.01                | 0.22       |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 20                  | 0.22     | 0.01                | 0.22       |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 20                  | 0.22     | 0.01                | 0.22       |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG12  | 20                  | 0.22     | 0.01                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG23 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG21 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG21 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG21 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG22 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG23 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG23 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG22 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG23 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,403)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG21 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG21 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG21 | 20                  | 0.22     | 0.04                | 0.22       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG22 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG23 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,403)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG23 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG22 | 20                  | 0.22     | 0.04                | 0.22       |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 20                  | 0.21     | 0.03                | 0.21       |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 20                  | 0.21     | 0.03                | 0.22       |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG23 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG21 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG23 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG21 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,395)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG13 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,395)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG13 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,396)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG13 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,396)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG13 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG22  | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG21  | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG23  | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG22  | 20                  | 0.15     | 0.01                | 0.15       |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG21  | 20                  | 0.15     | 0.01                | 0.15       |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG23  | 20                  | 0.15     | 0.01                | 0.15       |
| (1,967)  | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 20                  | 0.15     | 0.0                 | 0.15       |
| (1,968)  | 1:32:B:LYS:HG3   | 1:32:B:LYS:HG2   | 20                  | 0.15     | 0.0                 | 0.15       |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 20                  | 0.14     | 0.0                 | 0.14       |
| (1,538)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HG2  | 20                  | 0.14     | 0.0                 | 0.14       |
| (1,165)  | 1:35:A:GLU:HG2   | 1:35:A:GLU:HG3   | 20                  | 0.13     | 0.0                 | 0.13       |
| (1,166)  | 1:35:B:GLU:HG2   | 1:35:B:GLU:HG3   | 20                  | 0.13     | 0.0                 | 0.13       |
| (1,333)  | 1:36:A:VAL:HG12  | 1:36:A:VAL:HB    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,333)  | 1:36:A:VAL:HG11  | 1:36:A:VAL:HB    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,333)  | 1:36:A:VAL:HG13  | 1:36:A:VAL:HB    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,334)  | 1:36:B:VAL:HG12  | 1:36:B:VAL:HB    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,334)  | 1:36:B:VAL:HG11  | 1:36:B:VAL:HB    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,334)  | 1:36:B:VAL:HG13  | 1:36:B:VAL:HB    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,1023) | 1:13:A:SER:HB3   | 1:13:A:SER:HB2   | 20                  | 0.12     | 0.0                 | 0.12       |
| (1,1024) | 1:13:B:SER:HB3   | 1:13:B:SER:HB2   | 20                  | 0.12     | 0.0                 | 0.12       |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD22 | 19                  | 1.83     | 0.76                | 1.79       |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD21 | 19                  | 1.83     | 0.76                | 1.79       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2544) | 1:76:B:TRP:HE1  | 1:112:B:LEU:HD23 | 19                  | 1.83     | 0.76                | 1.79       |
| (1,2543) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HD22 | 19                  | 1.83     | 0.76                | 1.79       |
| (1,2543) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HD21 | 19                  | 1.83     | 0.76                | 1.79       |
| (1,2543) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HD23 | 19                  | 1.83     | 0.76                | 1.79       |
| (1,544)  | 1:92:B:MET:HE2  | 1:39:B:LEU:HD21  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE2  | 1:39:B:LEU:HD23  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE3  | 1:39:B:LEU:HD21  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE1  | 1:39:B:LEU:HD23  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE1  | 1:39:B:LEU:HD22  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE3  | 1:39:B:LEU:HD23  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE1  | 1:39:B:LEU:HD21  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE2  | 1:39:B:LEU:HD22  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,544)  | 1:92:B:MET:HE3  | 1:39:B:LEU:HD22  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE2  | 1:39:A:LEU:HD21  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE2  | 1:39:A:LEU:HD23  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE3  | 1:39:A:LEU:HD21  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE1  | 1:39:A:LEU:HD23  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE1  | 1:39:A:LEU:HD22  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE3  | 1:39:A:LEU:HD23  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE1  | 1:39:A:LEU:HD21  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE2  | 1:39:A:LEU:HD22  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,543)  | 1:92:A:MET:HE3  | 1:39:A:LEU:HD22  | 19                  | 1.61     | 0.64                | 1.66       |
| (1,2149) | 1:77:A:ASN:H    | 1:112:A:LEU:HD21 | 19                  | 1.35     | 0.36                | 1.38       |
| (1,2149) | 1:77:A:ASN:H    | 1:112:A:LEU:HD22 | 19                  | 1.35     | 0.36                | 1.38       |
| (1,2149) | 1:77:A:ASN:H    | 1:112:A:LEU:HD23 | 19                  | 1.35     | 0.36                | 1.38       |
| (1,2150) | 1:77:B:ASN:H    | 1:112:B:LEU:HD21 | 19                  | 1.34     | 0.36                | 1.38       |
| (1,2150) | 1:77:B:ASN:H    | 1:112:B:LEU:HD22 | 19                  | 1.34     | 0.36                | 1.38       |
| (1,2150) | 1:77:B:ASN:H    | 1:112:B:LEU:HD23 | 19                  | 1.34     | 0.36                | 1.38       |
| (1,3095) | 1:69:A:ARG:HA   | 1:112:B:LEU:HD23 | 19                  | 1.21     | 0.91                | 0.97       |
| (1,3095) | 1:69:A:ARG:HA   | 1:112:B:LEU:HD22 | 19                  | 1.21     | 0.91                | 0.97       |
| (1,3095) | 1:69:A:ARG:HA   | 1:112:B:LEU:HD21 | 19                  | 1.21     | 0.91                | 0.97       |
| (1,3096) | 1:69:B:ARG:HA   | 1:112:A:LEU:HD23 | 19                  | 1.2      | 0.91                | 1.0        |
| (1,3096) | 1:69:B:ARG:HA   | 1:112:A:LEU:HD22 | 19                  | 1.2      | 0.91                | 1.0        |
| (1,3096) | 1:69:B:ARG:HA   | 1:112:A:LEU:HD21 | 19                  | 1.2      | 0.91                | 1.0        |
| (1,960)  | 1:59:B:ARG:HD2  | 1:18:B:VAL:HB    | 19                  | 1.11     | 0.86                | 0.69       |
| (1,959)  | 1:59:A:ARG:HD2  | 1:18:A:VAL:HB    | 19                  | 1.11     | 0.86                | 0.68       |
| (1,661)  | 1:42:A:VAL:HG13 | 1:90:A:LEU:HG    | 19                  | 0.81     | 0.4                 | 0.7        |
| (1,661)  | 1:42:A:VAL:HG11 | 1:90:A:LEU:HG    | 19                  | 0.81     | 0.4                 | 0.7        |
| (1,661)  | 1:42:A:VAL:HG12 | 1:90:A:LEU:HG    | 19                  | 0.81     | 0.4                 | 0.7        |
| (1,662)  | 1:42:B:VAL:HG13 | 1:90:B:LEU:HG    | 19                  | 0.81     | 0.4                 | 0.7        |
| (1,662)  | 1:42:B:VAL:HG11 | 1:90:B:LEU:HG    | 19                  | 0.81     | 0.4                 | 0.7        |
| (1,662)  | 1:42:B:VAL:HG12 | 1:90:B:LEU:HG    | 19                  | 0.81     | 0.4                 | 0.7        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2186) | 1:100:B:ARG:H   | 1:98:B:ALA:HB2  | 19                  | 0.8      | 0.23                | 0.75       |
| (1,2186) | 1:100:B:ARG:H   | 1:98:B:ALA:HB3  | 19                  | 0.8      | 0.23                | 0.75       |
| (1,2186) | 1:100:B:ARG:H   | 1:98:B:ALA:HB1  | 19                  | 0.8      | 0.23                | 0.75       |
| (1,2185) | 1:100:A:ARG:H   | 1:98:A:ALA:HB2  | 19                  | 0.8      | 0.23                | 0.75       |
| (1,2185) | 1:100:A:ARG:H   | 1:98:A:ALA:HB3  | 19                  | 0.8      | 0.23                | 0.75       |
| (1,2185) | 1:100:A:ARG:H   | 1:98:A:ALA:HB1  | 19                  | 0.8      | 0.23                | 0.75       |
| (1,1388) | 1:20:B:VAL:HG11 | 1:19:B:SER:H    | 19                  | 0.66     | 0.3                 | 0.56       |
| (1,1388) | 1:20:B:VAL:HG13 | 1:19:B:SER:H    | 19                  | 0.66     | 0.3                 | 0.56       |
| (1,1388) | 1:20:B:VAL:HG12 | 1:19:B:SER:H    | 19                  | 0.66     | 0.3                 | 0.56       |
| (1,1387) | 1:20:A:VAL:HG11 | 1:19:A:SER:H    | 19                  | 0.65     | 0.3                 | 0.57       |
| (1,1387) | 1:20:A:VAL:HG13 | 1:19:A:SER:H    | 19                  | 0.65     | 0.3                 | 0.57       |
| (1,1387) | 1:20:A:VAL:HG12 | 1:19:A:SER:H    | 19                  | 0.65     | 0.3                 | 0.57       |
| (1,583)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HD2 | 19                  | 0.54     | 0.37                | 0.5        |
| (1,584)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HD2 | 19                  | 0.54     | 0.37                | 0.51       |
| (1,2906) | 1:22:B:VAL:H    | 1:53:B:PHE:HB3  | 19                  | 0.38     | 0.18                | 0.36       |
| (1,2905) | 1:22:A:VAL:H    | 1:53:A:PHE:HB3  | 19                  | 0.38     | 0.18                | 0.36       |
| (1,237)  | 1:55:A:GLU:H    | 1:20:A:VAL:HA   | 19                  | 0.3      | 0.1                 | 0.27       |
| (1,238)  | 1:55:B:GLU:H    | 1:20:B:VAL:HA   | 19                  | 0.3      | 0.1                 | 0.28       |
| (1,1172) | 1:39:B:LEU:HD21 | 1:92:B:MET:HG2  | 18                  | 1.28     | 1.07                | 1.08       |
| (1,1172) | 1:39:B:LEU:HD23 | 1:92:B:MET:HG2  | 18                  | 1.28     | 1.07                | 1.08       |
| (1,1172) | 1:39:B:LEU:HD22 | 1:92:B:MET:HG2  | 18                  | 1.28     | 1.07                | 1.08       |
| (1,1171) | 1:39:A:LEU:HD21 | 1:92:A:MET:HG2  | 18                  | 1.28     | 1.07                | 1.08       |
| (1,1171) | 1:39:A:LEU:HD23 | 1:92:A:MET:HG2  | 18                  | 1.28     | 1.07                | 1.08       |
| (1,1171) | 1:39:A:LEU:HD22 | 1:92:A:MET:HG2  | 18                  | 1.28     | 1.07                | 1.08       |
| (1,2598) | 1:107:B:ALA:H   | 1:108:B:CYS:HB3 | 18                  | 0.65     | 0.2                 | 0.68       |
| (1,2597) | 1:107:A:ALA:H   | 1:108:A:CYS:HB3 | 18                  | 0.65     | 0.19                | 0.68       |
| (1,65)   | 1:32:A:LYS:HE2  | 1:32:A:LYS:HD2  | 18                  | 0.6      | 0.17                | 0.66       |
| (1,66)   | 1:32:B:LYS:HE2  | 1:32:B:LYS:HD2  | 18                  | 0.6      | 0.17                | 0.66       |
| (1,2384) | 1:29:B:THR:H    | 1:30:B:ASP:HB2  | 18                  | 0.53     | 0.33                | 0.5        |
| (1,2221) | 1:118:A:ARG:H   | 1:117:A:VAL:HB  | 18                  | 0.45     | 0.16                | 0.43       |
| (1,2222) | 1:118:B:ARG:H   | 1:117:B:VAL:HB  | 18                  | 0.45     | 0.16                | 0.42       |
| (1,3028) | 1:35:B:GLU:H    | 1:36:B:VAL:HG11 | 18                  | 0.45     | 0.1                 | 0.46       |
| (1,3028) | 1:35:B:GLU:H    | 1:36:B:VAL:HG13 | 18                  | 0.45     | 0.1                 | 0.46       |
| (1,3028) | 1:35:B:GLU:H    | 1:36:B:VAL:HG12 | 18                  | 0.45     | 0.1                 | 0.46       |
| (1,3027) | 1:35:A:GLU:H    | 1:36:A:VAL:HG11 | 18                  | 0.44     | 0.1                 | 0.46       |
| (1,3027) | 1:35:A:GLU:H    | 1:36:A:VAL:HG13 | 18                  | 0.44     | 0.1                 | 0.46       |
| (1,3027) | 1:35:A:GLU:H    | 1:36:A:VAL:HG12 | 18                  | 0.44     | 0.1                 | 0.46       |
| (1,343)  | 1:48:A:VAL:HG11 | 1:41:A:GLU:HG2  | 17                  | 1.43     | 1.38                | 0.68       |
| (1,343)  | 1:48:A:VAL:HG13 | 1:41:A:GLU:HG2  | 17                  | 1.43     | 1.38                | 0.68       |
| (1,343)  | 1:48:A:VAL:HG12 | 1:41:A:GLU:HG2  | 17                  | 1.43     | 1.38                | 0.68       |
| (1,344)  | 1:48:B:VAL:HG11 | 1:41:B:GLU:HG2  | 17                  | 1.43     | 1.38                | 0.69       |
| (1,344)  | 1:48:B:VAL:HG13 | 1:41:B:GLU:HG2  | 17                  | 1.43     | 1.38                | 0.69       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,344)  | 1:48:B:VAL:HG12 | 1:41:B:GLU:HG2  | 17                  | 1.43     | 1.38                | 0.69       |
| (1,1399) | 1:59:A:ARG:HG2  | 1:18:A:VAL:HG13 | 17                  | 1.26     | 0.65                | 1.48       |
| (1,1399) | 1:59:A:ARG:HG2  | 1:18:A:VAL:HG12 | 17                  | 1.26     | 0.65                | 1.48       |
| (1,1399) | 1:59:A:ARG:HG2  | 1:18:A:VAL:HG11 | 17                  | 1.26     | 0.65                | 1.48       |
| (1,1400) | 1:59:B:ARG:HG2  | 1:18:B:VAL:HG13 | 17                  | 1.26     | 0.65                | 1.48       |
| (1,1400) | 1:59:B:ARG:HG2  | 1:18:B:VAL:HG12 | 17                  | 1.26     | 0.65                | 1.48       |
| (1,1400) | 1:59:B:ARG:HG2  | 1:18:B:VAL:HG11 | 17                  | 1.26     | 0.65                | 1.48       |
| (1,548)  | 1:92:B:MET:HE2  | 1:92:B:MET:HB2  | 17                  | 0.84     | 0.13                | 0.9        |
| (1,548)  | 1:92:B:MET:HE1  | 1:92:B:MET:HB2  | 17                  | 0.84     | 0.13                | 0.9        |
| (1,548)  | 1:92:B:MET:HE3  | 1:92:B:MET:HB2  | 17                  | 0.84     | 0.13                | 0.9        |
| (1,547)  | 1:92:A:MET:HE2  | 1:92:A:MET:HB2  | 17                  | 0.84     | 0.13                | 0.9        |
| (1,547)  | 1:92:A:MET:HE1  | 1:92:A:MET:HB2  | 17                  | 0.84     | 0.13                | 0.9        |
| (1,547)  | 1:92:A:MET:HE3  | 1:92:A:MET:HB2  | 17                  | 0.84     | 0.13                | 0.9        |
| (1,1063) | 1:57:A:LYS:HD2  | 1:57:A:LYS:HB2  | 17                  | 0.74     | 0.46                | 0.67       |
| (1,1064) | 1:57:B:LYS:HD2  | 1:57:B:LYS:HB2  | 17                  | 0.74     | 0.45                | 0.67       |
| (1,2613) | 1:19:A:SER:H    | 1:18:A:VAL:HG22 | 17                  | 0.64     | 0.26                | 0.61       |
| (1,2613) | 1:19:A:SER:H    | 1:18:A:VAL:HG21 | 17                  | 0.64     | 0.26                | 0.61       |
| (1,2613) | 1:19:A:SER:H    | 1:18:A:VAL:HG23 | 17                  | 0.64     | 0.26                | 0.61       |
| (1,2614) | 1:19:B:SER:H    | 1:18:B:VAL:HG22 | 17                  | 0.64     | 0.26                | 0.61       |
| (1,2614) | 1:19:B:SER:H    | 1:18:B:VAL:HG21 | 17                  | 0.64     | 0.26                | 0.61       |
| (1,2614) | 1:19:B:SER:H    | 1:18:B:VAL:HG23 | 17                  | 0.64     | 0.26                | 0.61       |
| (1,681)  | 1:22:A:VAL:HB   | 1:53:A:PHE:HD1  | 17                  | 0.63     | 0.44                | 0.43       |
| (1,682)  | 1:22:B:VAL:HB   | 1:53:B:PHE:HD1  | 17                  | 0.63     | 0.44                | 0.44       |
| (1,2383) | 1:29:A:THR:H    | 1:30:A:ASP:HB2  | 17                  | 0.55     | 0.33                | 0.74       |
| (1,47)   | 1:42:A:VAL:HG23 | 1:44:A:ILE:HB   | 17                  | 0.49     | 0.3                 | 0.42       |
| (1,47)   | 1:42:A:VAL:HG21 | 1:44:A:ILE:HB   | 17                  | 0.49     | 0.3                 | 0.42       |
| (1,47)   | 1:42:A:VAL:HG22 | 1:44:A:ILE:HB   | 17                  | 0.49     | 0.3                 | 0.42       |
| (1,48)   | 1:42:B:VAL:HG23 | 1:44:B:ILE:HB   | 17                  | 0.49     | 0.3                 | 0.42       |
| (1,48)   | 1:42:B:VAL:HG21 | 1:44:B:ILE:HB   | 17                  | 0.49     | 0.3                 | 0.42       |
| (1,48)   | 1:42:B:VAL:HG22 | 1:44:B:ILE:HB   | 17                  | 0.49     | 0.3                 | 0.42       |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB3 | 17                  | 0.19     | 0.05                | 0.2        |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB1 | 17                  | 0.19     | 0.05                | 0.2        |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB2 | 17                  | 0.19     | 0.05                | 0.2        |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB3 | 17                  | 0.19     | 0.05                | 0.2        |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB1 | 17                  | 0.19     | 0.05                | 0.2        |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB2 | 17                  | 0.19     | 0.05                | 0.2        |
| (1,3060) | 1:71:B:ILE:HD12 | 1:14:A:VAL:HB   | 16                  | 1.8      | 1.31                | 1.44       |
| (1,3060) | 1:71:B:ILE:HD13 | 1:14:A:VAL:HB   | 16                  | 1.8      | 1.31                | 1.44       |
| (1,3060) | 1:71:B:ILE:HD11 | 1:14:A:VAL:HB   | 16                  | 1.8      | 1.31                | 1.44       |
| (1,3059) | 1:71:A:ILE:HD12 | 1:14:B:VAL:HB   | 16                  | 1.8      | 1.32                | 1.46       |
| (1,3059) | 1:71:A:ILE:HD13 | 1:14:B:VAL:HB   | 16                  | 1.8      | 1.32                | 1.46       |
| (1,3059) | 1:71:A:ILE:HD11 | 1:14:B:VAL:HB   | 16                  | 1.8      | 1.32                | 1.46       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 16                  | 1.51     | 1.31                | 1.34       |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 16                  | 1.5      | 1.31                | 1.37       |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 16                  | 0.85     | 0.36                | 0.94       |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 16                  | 0.85     | 0.36                | 0.94       |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 16                  | 0.82     | 0.38                | 0.78       |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 16                  | 0.82     | 0.38                | 0.78       |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB3  | 16                  | 0.64     | 0.33                | 0.6        |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB1  | 16                  | 0.64     | 0.33                | 0.6        |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB2  | 16                  | 0.64     | 0.33                | 0.6        |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB3  | 16                  | 0.64     | 0.33                | 0.6        |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB1  | 16                  | 0.64     | 0.33                | 0.6        |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB2  | 16                  | 0.64     | 0.33                | 0.6        |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG22 | 16                  | 0.53     | 0.29                | 0.48       |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG23 | 16                  | 0.53     | 0.29                | 0.48       |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG21 | 16                  | 0.53     | 0.29                | 0.48       |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG22 | 16                  | 0.53     | 0.3                 | 0.5        |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 16                  | 0.53     | 0.3                 | 0.5        |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG21 | 16                  | 0.53     | 0.3                 | 0.5        |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG12 | 16                  | 0.4      | 0.25                | 0.32       |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG13 | 16                  | 0.4      | 0.25                | 0.32       |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG11 | 16                  | 0.4      | 0.25                | 0.32       |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2   | 16                  | 0.25     | 0.0                 | 0.25       |
| (1,484)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG2   | 16                  | 0.25     | 0.0                 | 0.25       |
| (1,3087) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HA    | 15                  | 1.14     | 0.8                 | 0.96       |
| (1,3087) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HA    | 15                  | 1.14     | 0.8                 | 0.96       |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 15                  | 1.14     | 0.8                 | 0.96       |
| (1,3088) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HA    | 15                  | 1.13     | 0.8                 | 0.96       |
| (1,3088) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HA    | 15                  | 1.13     | 0.8                 | 0.96       |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA    | 15                  | 1.13     | 0.8                 | 0.96       |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG12 | 15                  | 0.42     | 0.25                | 0.34       |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG13 | 15                  | 0.42     | 0.25                | 0.34       |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG11 | 15                  | 0.42     | 0.25                | 0.34       |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 15                  | 0.38     | 0.42                | 0.17       |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 15                  | 0.38     | 0.42                | 0.17       |
| (1,359)  | 1:41:A:GLU:HG2   | 1:41:A:GLU:HB2   | 15                  | 0.37     | 0.01                | 0.37       |
| (1,360)  | 1:41:B:GLU:HG2   | 1:41:B:GLU:HB2   | 15                  | 0.37     | 0.01                | 0.37       |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 15                  | 0.27     | 0.09                | 0.27       |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 15                  | 0.27     | 0.09                | 0.27       |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 15                  | 0.27     | 0.11                | 0.26       |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB1   | 15                  | 0.27     | 0.11                | 0.26       |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB3   | 15                  | 0.27     | 0.11                | 0.26       |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 15                  | 0.27     | 0.11                | 0.27       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2387) | 1:29:A:THR:H    | 1:28:A:ALA:HB1   | 15                  | 0.27     | 0.11                | 0.27       |
| (1,2387) | 1:29:A:THR:H    | 1:28:A:ALA:HB3   | 15                  | 0.27     | 0.11                | 0.27       |
| (3,16)   | 1:28:B:ALA:H    | 1:35:B:GLU:H     | 15                  | 0.26     | 0.05                | 0.26       |
| (3,16)   | 1:28:B:ALA:H    | 1:103:B:ARG:H    | 15                  | 0.26     | 0.05                | 0.26       |
| (3,15)   | 1:28:A:ALA:H    | 1:35:A:GLU:H     | 15                  | 0.26     | 0.05                | 0.26       |
| (3,15)   | 1:28:A:ALA:H    | 1:103:A:ARG:H    | 15                  | 0.26     | 0.05                | 0.26       |
| (1,1740) | 1:36:B:VAL:H    | 1:27:B:THR:HG21  | 15                  | 0.24     | 0.08                | 0.22       |
| (1,1740) | 1:36:B:VAL:H    | 1:27:B:THR:HG23  | 15                  | 0.24     | 0.08                | 0.22       |
| (1,1740) | 1:36:B:VAL:H    | 1:27:B:THR:HG22  | 15                  | 0.24     | 0.08                | 0.22       |
| (1,1739) | 1:36:A:VAL:H    | 1:27:A:THR:HG21  | 15                  | 0.24     | 0.09                | 0.23       |
| (1,1739) | 1:36:A:VAL:H    | 1:27:A:THR:HG23  | 15                  | 0.24     | 0.09                | 0.23       |
| (1,1739) | 1:36:A:VAL:H    | 1:27:A:THR:HG22  | 15                  | 0.24     | 0.09                | 0.23       |
| (1,1347) | 1:87:A:VAL:HG12 | 1:104:A:ILE:HD12 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1347) | 1:87:A:VAL:HG12 | 1:104:A:ILE:HD11 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1347) | 1:87:A:VAL:HG13 | 1:104:A:ILE:HD12 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1347) | 1:87:A:VAL:HG11 | 1:104:A:ILE:HD11 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1347) | 1:87:A:VAL:HG11 | 1:104:A:ILE:HD12 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1348) | 1:87:B:VAL:HG12 | 1:104:B:ILE:HD12 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1348) | 1:87:B:VAL:HG12 | 1:104:B:ILE:HD11 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1348) | 1:87:B:VAL:HG13 | 1:104:B:ILE:HD12 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1348) | 1:87:B:VAL:HG11 | 1:104:B:ILE:HD11 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,1348) | 1:87:B:VAL:HG11 | 1:104:B:ILE:HD12 | 15                  | 0.18     | 0.06                | 0.16       |
| (1,3099) | 1:9:A:ARG:HB3   | 1:117:B:VAL:HG23 | 14                  | 2.25     | 1.69                | 1.81       |
| (1,3099) | 1:9:A:ARG:HB3   | 1:117:B:VAL:HG22 | 14                  | 2.25     | 1.69                | 1.81       |
| (1,3099) | 1:9:A:ARG:HB2   | 1:117:B:VAL:HG23 | 14                  | 2.25     | 1.69                | 1.81       |
| (1,3099) | 1:9:A:ARG:HB2   | 1:117:B:VAL:HG22 | 14                  | 2.25     | 1.69                | 1.81       |
| (1,3099) | 1:9:A:ARG:HB3   | 1:117:B:VAL:HG21 | 14                  | 2.25     | 1.69                | 1.81       |
| (1,3099) | 1:9:A:ARG:HB2   | 1:117:B:VAL:HG21 | 14                  | 2.25     | 1.69                | 1.81       |
| (1,3100) | 1:9:B:ARG:HB3   | 1:117:A:VAL:HG23 | 14                  | 2.23     | 1.69                | 1.77       |
| (1,3100) | 1:9:B:ARG:HB3   | 1:117:A:VAL:HG22 | 14                  | 2.23     | 1.69                | 1.77       |
| (1,3100) | 1:9:B:ARG:HB2   | 1:117:A:VAL:HG23 | 14                  | 2.23     | 1.69                | 1.77       |
| (1,3100) | 1:9:B:ARG:HB2   | 1:117:A:VAL:HG22 | 14                  | 2.23     | 1.69                | 1.77       |
| (1,3100) | 1:9:B:ARG:HB3   | 1:117:A:VAL:HG21 | 14                  | 2.23     | 1.69                | 1.77       |
| (1,3100) | 1:9:B:ARG:HB2   | 1:117:A:VAL:HG21 | 14                  | 2.23     | 1.69                | 1.77       |
| (1,3076) | 1:42:B:VAL:HG23 | 1:99:A:TRP:HE1   | 14                  | 0.98     | 0.61                | 0.73       |
| (1,3076) | 1:42:B:VAL:HG21 | 1:99:A:TRP:HE1   | 14                  | 0.98     | 0.61                | 0.73       |
| (1,3076) | 1:42:B:VAL:HG22 | 1:99:A:TRP:HE1   | 14                  | 0.98     | 0.61                | 0.73       |
| (1,3075) | 1:42:A:VAL:HG23 | 1:99:B:TRP:HE1   | 14                  | 0.97     | 0.61                | 0.7        |
| (1,3075) | 1:42:A:VAL:HG21 | 1:99:B:TRP:HE1   | 14                  | 0.97     | 0.61                | 0.7        |
| (1,3075) | 1:42:A:VAL:HG22 | 1:99:B:TRP:HE1   | 14                  | 0.97     | 0.61                | 0.7        |
| (1,311)  | 1:71:A:ILE:HG22 | 1:71:A:ILE:HG13  | 14                  | 0.81     | 0.02                | 0.8        |
| (1,311)  | 1:71:A:ILE:HG21 | 1:71:A:ILE:HG13  | 14                  | 0.81     | 0.02                | 0.8        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,311)  | 1:71:A:ILE:HG23  | 1:71:A:ILE:HG13  | 14                  | 0.81     | 0.02                | 0.8        |
| (1,312)  | 1:71:B:ILE:HG22  | 1:71:B:ILE:HG13  | 14                  | 0.8      | 0.02                | 0.8        |
| (1,312)  | 1:71:B:ILE:HG21  | 1:71:B:ILE:HG13  | 14                  | 0.8      | 0.02                | 0.8        |
| (1,312)  | 1:71:B:ILE:HG23  | 1:71:B:ILE:HG13  | 14                  | 0.8      | 0.02                | 0.8        |
| (1,249)  | 1:112:A:LEU:HD22 | 1:76:A:TRP:HD1   | 14                  | 0.8      | 0.56                | 0.64       |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 14                  | 0.8      | 0.56                | 0.64       |
| (1,249)  | 1:112:A:LEU:HD21 | 1:76:A:TRP:HD1   | 14                  | 0.8      | 0.56                | 0.64       |
| (1,250)  | 1:112:B:LEU:HD22 | 1:76:B:TRP:HD1   | 14                  | 0.8      | 0.56                | 0.64       |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 14                  | 0.8      | 0.56                | 0.64       |
| (1,250)  | 1:112:B:LEU:HD21 | 1:76:B:TRP:HD1   | 14                  | 0.8      | 0.56                | 0.64       |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 14                  | 0.54     | 0.37                | 0.37       |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 14                  | 0.54     | 0.37                | 0.36       |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 14                  | 0.26     | 0.21                | 0.18       |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 14                  | 0.26     | 0.21                | 0.18       |
| (1,1553) | 1:48:A:VAL:HG22  | 1:48:A:VAL:HB    | 14                  | 0.11     | 0.0                 | 0.11       |
| (1,1553) | 1:48:A:VAL:HG23  | 1:48:A:VAL:HB    | 14                  | 0.11     | 0.0                 | 0.11       |
| (1,1553) | 1:48:A:VAL:HG21  | 1:48:A:VAL:HB    | 14                  | 0.11     | 0.0                 | 0.11       |
| (1,3102) | 1:9:B:ARG:HB3    | 1:115:A:LYS:HA   | 13                  | 1.82     | 1.53                | 1.63       |
| (1,3102) | 1:9:B:ARG:HB2    | 1:115:A:LYS:HA   | 13                  | 1.82     | 1.53                | 1.63       |
| (1,3101) | 1:9:A:ARG:HB3    | 1:115:B:LYS:HA   | 13                  | 1.82     | 1.52                | 1.59       |
| (1,3101) | 1:9:A:ARG:HB2    | 1:115:B:LYS:HA   | 13                  | 1.82     | 1.52                | 1.59       |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 13                  | 1.68     | 1.03                | 1.64       |
| (1,3057) | 1:70:A:GLY:HA3   | 1:76:B:TRP:HE1   | 13                  | 1.68     | 1.03                | 1.64       |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 13                  | 1.67     | 1.03                | 1.64       |
| (1,3058) | 1:70:B:GLY:HA3   | 1:76:A:TRP:HE1   | 13                  | 1.67     | 1.03                | 1.64       |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 13                  | 1.61     | 0.21                | 1.61       |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 13                  | 1.61     | 0.21                | 1.61       |
| (1,251)  | 1:112:A:LEU:HD21 | 1:71:A:ILE:HA    | 13                  | 1.13     | 0.67                | 1.19       |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 13                  | 1.13     | 0.67                | 1.19       |
| (1,251)  | 1:112:A:LEU:HD22 | 1:71:A:ILE:HA    | 13                  | 1.13     | 0.67                | 1.19       |
| (1,252)  | 1:112:B:LEU:HD21 | 1:71:B:ILE:HA    | 13                  | 1.13     | 0.67                | 1.19       |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 13                  | 1.13     | 0.67                | 1.19       |
| (1,252)  | 1:112:B:LEU:HD22 | 1:71:B:ILE:HA    | 13                  | 1.13     | 0.67                | 1.19       |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG11 | 13                  | 1.13     | 0.72                | 0.81       |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG13 | 13                  | 1.13     | 0.72                | 0.81       |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG12 | 13                  | 1.13     | 0.72                | 0.81       |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG11 | 13                  | 1.13     | 0.72                | 0.82       |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG13 | 13                  | 1.13     | 0.72                | 0.82       |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG12 | 13                  | 1.13     | 0.72                | 0.82       |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 13                  | 0.63     | 0.09                | 0.64       |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 13                  | 0.63     | 0.09                | 0.63       |
| (1,3056) | 1:107:B:ALA:HB3  | 1:109:A:VAL:HG13 | 13                  | 0.57     | 0.32                | 0.42       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3056) | 1:107:B:ALA:HB3 | 1:109:A:VAL:HG12 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3056) | 1:107:B:ALA:HB2 | 1:109:A:VAL:HG12 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3056) | 1:107:B:ALA:HB2 | 1:109:A:VAL:HG11 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3056) | 1:107:B:ALA:HB1 | 1:109:A:VAL:HG13 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3056) | 1:107:B:ALA:HB2 | 1:109:A:VAL:HG13 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3056) | 1:107:B:ALA:HB1 | 1:109:A:VAL:HG11 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3056) | 1:107:B:ALA:HB3 | 1:109:A:VAL:HG11 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3056) | 1:107:B:ALA:HB1 | 1:109:A:VAL:HG12 | 13                  | 0.57     | 0.32                | 0.42       |
| (1,3055) | 1:107:A:ALA:HB3 | 1:109:B:VAL:HG13 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB3 | 1:109:B:VAL:HG12 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB2 | 1:109:B:VAL:HG12 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB2 | 1:109:B:VAL:HG11 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB1 | 1:109:B:VAL:HG13 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB2 | 1:109:B:VAL:HG13 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB1 | 1:109:B:VAL:HG11 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB3 | 1:109:B:VAL:HG11 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3055) | 1:107:A:ALA:HB1 | 1:109:B:VAL:HG12 | 13                  | 0.57     | 0.34                | 0.41       |
| (1,3004) | 1:28:B:ALA:H    | 1:38:B:VAL:HG11  | 13                  | 0.31     | 0.19                | 0.23       |
| (1,3004) | 1:28:B:ALA:H    | 1:38:B:VAL:HG13  | 13                  | 0.31     | 0.19                | 0.23       |
| (1,3004) | 1:28:B:ALA:H    | 1:38:B:VAL:HG12  | 13                  | 0.31     | 0.19                | 0.23       |
| (1,3003) | 1:28:A:ALA:H    | 1:38:A:VAL:HG11  | 13                  | 0.31     | 0.19                | 0.23       |
| (1,3003) | 1:28:A:ALA:H    | 1:38:A:VAL:HG13  | 13                  | 0.31     | 0.19                | 0.23       |
| (1,3003) | 1:28:A:ALA:H    | 1:38:A:VAL:HG12  | 13                  | 0.31     | 0.19                | 0.23       |
| (1,988)  | 1:27:B:THR:HG21 | 1:35:B:GLU:HG3   | 13                  | 0.27     | 0.12                | 0.24       |
| (1,988)  | 1:27:B:THR:HG22 | 1:35:B:GLU:HG3   | 13                  | 0.27     | 0.12                | 0.24       |
| (1,988)  | 1:27:B:THR:HG23 | 1:35:B:GLU:HG3   | 13                  | 0.27     | 0.12                | 0.24       |
| (1,987)  | 1:27:A:THR:HG21 | 1:35:A:GLU:HG3   | 13                  | 0.27     | 0.12                | 0.24       |
| (1,987)  | 1:27:A:THR:HG22 | 1:35:A:GLU:HG3   | 13                  | 0.27     | 0.12                | 0.24       |
| (1,987)  | 1:27:A:THR:HG23 | 1:35:A:GLU:HG3   | 13                  | 0.27     | 0.12                | 0.24       |
| (1,1443) | 1:25:A:LYS:HD2  | 1:25:A:LYS:HG2   | 13                  | 0.26     | 0.0                 | 0.26       |
| (1,1444) | 1:25:B:LYS:HD2  | 1:25:B:LYS:HG2   | 13                  | 0.26     | 0.0                 | 0.26       |
| (1,1554) | 1:48:B:VAL:HG22 | 1:48:B:VAL:HB    | 13                  | 0.11     | 0.0                 | 0.11       |
| (1,1554) | 1:48:B:VAL:HG23 | 1:48:B:VAL:HB    | 13                  | 0.11     | 0.0                 | 0.11       |
| (1,1554) | 1:48:B:VAL:HG21 | 1:48:B:VAL:HB    | 13                  | 0.11     | 0.0                 | 0.11       |
| (1,839)  | 1:36:A:VAL:HG12 | 1:37:A:MET:HG3   | 12                  | 0.94     | 0.11                | 0.92       |
| (1,839)  | 1:36:A:VAL:HG11 | 1:37:A:MET:HG3   | 12                  | 0.94     | 0.11                | 0.92       |
| (1,839)  | 1:36:A:VAL:HG13 | 1:37:A:MET:HG3   | 12                  | 0.94     | 0.11                | 0.92       |
| (1,840)  | 1:36:B:VAL:HG12 | 1:37:B:MET:HG3   | 12                  | 0.94     | 0.11                | 0.92       |
| (1,840)  | 1:36:B:VAL:HG11 | 1:37:B:MET:HG3   | 12                  | 0.94     | 0.11                | 0.92       |
| (1,840)  | 1:36:B:VAL:HG13 | 1:37:B:MET:HG3   | 12                  | 0.94     | 0.11                | 0.92       |
| (1,2853) | 1:73:A:SER:H    | 1:76:A:TRP:HB3   | 12                  | 0.87     | 0.74                | 0.57       |
| (1,2854) | 1:73:B:SER:H    | 1:76:B:TRP:HB3   | 12                  | 0.87     | 0.74                | 0.57       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3069) | 1:11:A:GLU:H    | 1:113:B:SER:HB3  | 12                  | 0.83     | 0.64                | 0.76       |
| (1,3069) | 1:11:A:GLU:H    | 1:113:B:SER:HB2  | 12                  | 0.83     | 0.64                | 0.76       |
| (1,1442) | 1:25:B:LYS:HG2  | 1:53:B:PHE:HD1   | 12                  | 0.79     | 0.53                | 0.47       |
| (1,1441) | 1:25:A:LYS:HG2  | 1:53:A:PHE:HD1   | 12                  | 0.79     | 0.53                | 0.46       |
| (1,587)  | 1:115:A:LYS:HD2 | 1:115:A:LYS:HB3  | 12                  | 0.52     | 0.24                | 0.44       |
| (1,588)  | 1:115:B:LYS:HD2 | 1:115:B:LYS:HB3  | 12                  | 0.52     | 0.24                | 0.45       |
| (1,511)  | 1:37:A:MET:HG2  | 1:37:A:MET:HE1   | 12                  | 0.41     | 0.01                | 0.41       |
| (1,511)  | 1:37:A:MET:HG2  | 1:37:A:MET:HE3   | 12                  | 0.41     | 0.01                | 0.41       |
| (1,511)  | 1:37:A:MET:HG2  | 1:37:A:MET:HE2   | 12                  | 0.41     | 0.01                | 0.41       |
| (1,512)  | 1:37:B:MET:HG2  | 1:37:B:MET:HE1   | 12                  | 0.41     | 0.01                | 0.41       |
| (1,512)  | 1:37:B:MET:HG2  | 1:37:B:MET:HE3   | 12                  | 0.41     | 0.01                | 0.41       |
| (1,512)  | 1:37:B:MET:HG2  | 1:37:B:MET:HE2   | 12                  | 0.41     | 0.01                | 0.41       |
| (1,1701) | 1:31:A:ILE:H    | 1:102:A:ILE:HG23 | 12                  | 0.27     | 0.15                | 0.2        |
| (1,1701) | 1:31:A:ILE:H    | 1:102:A:ILE:HG21 | 12                  | 0.27     | 0.15                | 0.2        |
| (1,1701) | 1:31:A:ILE:H    | 1:102:A:ILE:HG22 | 12                  | 0.27     | 0.15                | 0.2        |
| (1,1702) | 1:31:B:ILE:H    | 1:102:B:ILE:HG23 | 12                  | 0.27     | 0.15                | 0.2        |
| (1,1702) | 1:31:B:ILE:H    | 1:102:B:ILE:HG21 | 12                  | 0.27     | 0.15                | 0.2        |
| (1,1702) | 1:31:B:ILE:H    | 1:102:B:ILE:HG22 | 12                  | 0.27     | 0.15                | 0.2        |
| (1,1911) | 1:72:A:ASP:H    | 1:76:A:TRP:HB3   | 11                  | 1.34     | 1.39                | 0.87       |
| (1,1912) | 1:72:B:ASP:H    | 1:76:B:TRP:HB3   | 11                  | 1.34     | 1.39                | 0.87       |
| (1,1952) | 1:105:B:ASP:H   | 1:55:B:GLU:HB2   | 11                  | 1.28     | 0.59                | 1.25       |
| (1,1951) | 1:105:A:ASP:H   | 1:55:A:GLU:HB2   | 11                  | 1.27     | 0.6                 | 1.25       |
| (1,61)   | 1:63:A:PRO:HD2  | 1:64:A:VAL:HG12  | 11                  | 1.16     | 0.58                | 1.09       |
| (1,61)   | 1:63:A:PRO:HD2  | 1:64:A:VAL:HG13  | 11                  | 1.16     | 0.58                | 1.09       |
| (1,61)   | 1:63:A:PRO:HD2  | 1:64:A:VAL:HG11  | 11                  | 1.16     | 0.58                | 1.09       |
| (1,62)   | 1:63:B:PRO:HD2  | 1:64:B:VAL:HG12  | 11                  | 1.16     | 0.58                | 1.1        |
| (1,62)   | 1:63:B:PRO:HD2  | 1:64:B:VAL:HG13  | 11                  | 1.16     | 0.58                | 1.1        |
| (1,62)   | 1:63:B:PRO:HD2  | 1:64:B:VAL:HG11  | 11                  | 1.16     | 0.58                | 1.1        |
| (3,8)    | 1:79:B:TYR:H    | 1:71:B:ILE:HD12  | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,8)    | 1:79:B:TYR:H    | 1:71:B:ILE:HD11  | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,8)    | 1:79:B:TYR:H    | 1:71:B:ILE:HD13  | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,8)    | 1:79:B:TYR:H    | 1:112:B:LEU:HD21 | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,8)    | 1:79:B:TYR:H    | 1:112:B:LEU:HD22 | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,8)    | 1:79:B:TYR:H    | 1:112:B:LEU:HD23 | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,7)    | 1:79:A:TYR:H    | 1:71:A:ILE:HD12  | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,7)    | 1:79:A:TYR:H    | 1:71:A:ILE:HD11  | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,7)    | 1:79:A:TYR:H    | 1:71:A:ILE:HD13  | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,7)    | 1:79:A:TYR:H    | 1:112:A:LEU:HD21 | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,7)    | 1:79:A:TYR:H    | 1:112:A:LEU:HD22 | 11                  | 1.01     | 0.9                 | 0.61       |
| (3,7)    | 1:79:A:TYR:H    | 1:112:A:LEU:HD23 | 11                  | 1.01     | 0.9                 | 0.61       |
| (1,2547) | 1:76:A:TRP:HE1  | 1:71:A:ILE:HG23  | 11                  | 0.92     | 0.48                | 1.08       |
| (1,2547) | 1:76:A:TRP:HE1  | 1:71:A:ILE:HG22  | 11                  | 0.92     | 0.48                | 1.08       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2547) | 1:76:A:TRP:HE1  | 1:71:A:ILE:HG21  | 11                  | 0.92     | 0.48                | 1.08       |
| (1,2548) | 1:76:B:TRP:HE1  | 1:71:B:ILE:HG23  | 11                  | 0.91     | 0.47                | 1.07       |
| (1,2548) | 1:76:B:TRP:HE1  | 1:71:B:ILE:HG22  | 11                  | 0.91     | 0.47                | 1.07       |
| (1,2548) | 1:76:B:TRP:HE1  | 1:71:B:ILE:HG21  | 11                  | 0.91     | 0.47                | 1.07       |
| (1,3070) | 1:11:B:GLU:H    | 1:113:A:SER:HB3  | 11                  | 0.91     | 0.63                | 0.82       |
| (1,3070) | 1:11:B:GLU:H    | 1:113:A:SER:HB2  | 11                  | 0.91     | 0.63                | 0.82       |
| (1,1251) | 1:68:A:CYS:HB3  | 1:14:A:VAL:HB    | 11                  | 0.87     | 0.91                | 0.72       |
| (1,1252) | 1:68:B:CYS:HB3  | 1:14:B:VAL:HB    | 11                  | 0.87     | 0.91                | 0.72       |
| (1,461)  | 1:44:A:ILE:HG12 | 1:43:A:ASN:HB2   | 11                  | 0.84     | 0.2                 | 0.89       |
| (1,462)  | 1:44:B:ILE:HG12 | 1:43:B:ASN:HB2   | 11                  | 0.84     | 0.21                | 0.88       |
| (1,1538) | 1:18:B:VAL:H    | 1:57:B:LYS:HG2   | 11                  | 0.77     | 0.18                | 0.79       |
| (1,1537) | 1:18:A:VAL:H    | 1:57:A:LYS:HG2   | 11                  | 0.77     | 0.18                | 0.79       |
| (1,1215) | 1:22:A:VAL:HG11 | 1:20:A:VAL:HB    | 11                  | 0.67     | 0.47                | 0.5        |
| (1,1215) | 1:22:A:VAL:HG13 | 1:20:A:VAL:HB    | 11                  | 0.67     | 0.47                | 0.5        |
| (1,1215) | 1:22:A:VAL:HG12 | 1:20:A:VAL:HB    | 11                  | 0.67     | 0.47                | 0.5        |
| (1,1216) | 1:22:B:VAL:HG11 | 1:20:B:VAL:HB    | 11                  | 0.67     | 0.47                | 0.5        |
| (1,1216) | 1:22:B:VAL:HG13 | 1:20:B:VAL:HB    | 11                  | 0.67     | 0.47                | 0.5        |
| (1,1216) | 1:22:B:VAL:HG12 | 1:20:B:VAL:HB    | 11                  | 0.67     | 0.47                | 0.5        |
| (1,459)  | 1:43:A:ASN:HB3  | 1:44:A:ILE:HG12  | 11                  | 0.41     | 0.19                | 0.39       |
| (1,460)  | 1:43:B:ASN:HB3  | 1:44:B:ILE:HG12  | 11                  | 0.41     | 0.19                | 0.39       |
| (1,5)    | 1:79:A:TYR:H    | 1:111:A:VAL:HG23 | 11                  | 0.34     | 0.16                | 0.3        |
| (1,5)    | 1:79:A:TYR:H    | 1:111:A:VAL:HG21 | 11                  | 0.34     | 0.16                | 0.3        |
| (1,5)    | 1:79:A:TYR:H    | 1:111:A:VAL:HG22 | 11                  | 0.34     | 0.16                | 0.3        |
| (1,6)    | 1:79:B:TYR:H    | 1:111:B:VAL:HG23 | 11                  | 0.33     | 0.16                | 0.3        |
| (1,6)    | 1:79:B:TYR:H    | 1:111:B:VAL:HG21 | 11                  | 0.33     | 0.16                | 0.3        |
| (1,6)    | 1:79:B:TYR:H    | 1:111:B:VAL:HG22 | 11                  | 0.33     | 0.16                | 0.3        |
| (1,2224) | 1:118:B:ARG:H   | 1:118:B:ARG:HB2  | 11                  | 0.3      | 0.12                | 0.26       |
| (1,2223) | 1:118:A:ARG:H   | 1:118:A:ARG:HB2  | 11                  | 0.29     | 0.12                | 0.27       |
| (1,416)  | 1:39:B:LEU:H    | 1:38:B:VAL:HG13  | 11                  | 0.28     | 0.12                | 0.23       |
| (1,416)  | 1:39:B:LEU:H    | 1:38:B:VAL:HG12  | 11                  | 0.28     | 0.12                | 0.23       |
| (1,416)  | 1:39:B:LEU:H    | 1:38:B:VAL:HG11  | 11                  | 0.28     | 0.12                | 0.23       |
| (1,415)  | 1:39:A:LEU:H    | 1:38:A:VAL:HG13  | 11                  | 0.28     | 0.12                | 0.23       |
| (1,415)  | 1:39:A:LEU:H    | 1:38:A:VAL:HG12  | 11                  | 0.28     | 0.12                | 0.23       |
| (1,415)  | 1:39:A:LEU:H    | 1:38:A:VAL:HG11  | 11                  | 0.28     | 0.12                | 0.23       |
| (1,711)  | 1:34:A:LYS:HB2  | 1:34:A:LYS:HD2   | 11                  | 0.14     | 0.03                | 0.13       |
| (1,912)  | 1:9:B:ARG:HB2   | 1:6:B:ILE:HG13   | 10                  | 1.76     | 1.74                | 1.04       |
| (1,911)  | 1:9:A:ARG:HB2   | 1:6:A:ILE:HG13   | 10                  | 1.76     | 1.74                | 1.04       |
| (1,270)  | 1:14:B:VAL:HG11 | 1:110:B:CYS:HB3  | 10                  | 1.36     | 0.77                | 1.2        |
| (1,270)  | 1:14:B:VAL:HG12 | 1:110:B:CYS:HB3  | 10                  | 1.36     | 0.77                | 1.2        |
| (1,270)  | 1:14:B:VAL:HG13 | 1:110:B:CYS:HB3  | 10                  | 1.36     | 0.77                | 1.2        |
| (1,269)  | 1:14:A:VAL:HG11 | 1:110:A:CYS:HB3  | 10                  | 1.35     | 0.77                | 1.2        |
| (1,269)  | 1:14:A:VAL:HG12 | 1:110:A:CYS:HB3  | 10                  | 1.35     | 0.77                | 1.2        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,269)  | 1:14:A:VAL:HG13 | 1:110:A:CYS:HB3 | 10                  | 1.35     | 0.77                | 1.2        |
| (1,1721) | 1:76:A:TRP:H    | 1:115:A:LYS:HG2 | 10                  | 0.86     | 0.83                | 0.57       |
| (1,1722) | 1:76:B:TRP:H    | 1:115:B:LYS:HG2 | 10                  | 0.86     | 0.83                | 0.56       |
| (1,2657) | 1:34:A:LYS:H    | 1:34:A:LYS:HG3  | 10                  | 0.51     | 0.02                | 0.51       |
| (1,2658) | 1:34:B:LYS:H    | 1:34:B:LYS:HG3  | 10                  | 0.51     | 0.02                | 0.51       |
| (1,1248) | 1:71:B:ILE:HG12 | 1:70:B:GLY:HA3  | 10                  | 0.44     | 0.23                | 0.4        |
| (1,1247) | 1:71:A:ILE:HG12 | 1:70:A:GLY:HA3  | 10                  | 0.43     | 0.23                | 0.4        |
| (1,2686) | 1:104:B:ILE:H   | 1:84:B:HIS:HB3  | 10                  | 0.4      | 0.12                | 0.41       |
| (1,2685) | 1:104:A:ILE:H   | 1:84:A:HIS:HB3  | 10                  | 0.4      | 0.12                | 0.42       |
| (1,585)  | 1:115:A:LYS:HD2 | 1:115:A:LYS:HG2 | 10                  | 0.22     | 0.0                 | 0.22       |
| (1,586)  | 1:115:B:LYS:HD2 | 1:115:B:LYS:HG2 | 10                  | 0.22     | 0.0                 | 0.22       |
| (1,805)  | 1:118:A:ARG:HG3 | 1:118:A:ARG:HB2 | 10                  | 0.21     | 0.02                | 0.22       |
| (1,806)  | 1:118:B:ARG:HG3 | 1:118:B:ARG:HB2 | 10                  | 0.21     | 0.02                | 0.22       |
| (1,2975) | 1:103:A:ARG:H   | 1:103:A:ARG:HG2 | 10                  | 0.2      | 0.06                | 0.18       |
| (1,2976) | 1:103:B:ARG:H   | 1:103:B:ARG:HG2 | 10                  | 0.19     | 0.06                | 0.18       |
| (1,853)  | 1:37:A:MET:HG3  | 1:36:A:VAL:HA   | 10                  | 0.17     | 0.04                | 0.17       |
| (1,854)  | 1:37:B:MET:HG3  | 1:36:B:VAL:HA   | 10                  | 0.17     | 0.04                | 0.17       |
| (1,712)  | 1:34:B:LYS:HB2  | 1:34:B:LYS:HD2  | 10                  | 0.14     | 0.03                | 0.14       |
| (1,2551) | 1:76:A:TRP:HE1  | 1:75:A:HIS:HB2  | 9                   | 2.13     | 1.17                | 1.52       |
| (1,2552) | 1:76:B:TRP:HE1  | 1:75:B:HIS:HB2  | 9                   | 2.12     | 1.17                | 1.52       |
| (1,1843) | 1:96:A:GLN:HE22 | 1:95:A:LYS:HA   | 9                   | 1.84     | 0.58                | 1.76       |
| (1,1844) | 1:96:B:GLN:HE22 | 1:95:B:LYS:HA   | 9                   | 1.84     | 0.57                | 1.75       |
| (1,908)  | 1:5:B:PRO:HA    | 1:9:B:ARG:HB2   | 9                   | 1.74     | 1.04                | 1.49       |
| (1,907)  | 1:5:A:PRO:HA    | 1:9:A:ARG:HB2   | 9                   | 1.74     | 1.04                | 1.48       |
| (1,3067) | 1:70:A:GLY:HA2  | 1:71:B:ILE:HG22 | 9                   | 1.54     | 1.26                | 0.83       |
| (1,3067) | 1:70:A:GLY:HA3  | 1:71:B:ILE:HG22 | 9                   | 1.54     | 1.26                | 0.83       |
| (1,3067) | 1:70:A:GLY:HA3  | 1:71:B:ILE:HG23 | 9                   | 1.54     | 1.26                | 0.83       |
| (1,3067) | 1:70:A:GLY:HA3  | 1:71:B:ILE:HG21 | 9                   | 1.54     | 1.26                | 0.83       |
| (1,3068) | 1:70:B:GLY:HA2  | 1:71:A:ILE:HG22 | 9                   | 1.52     | 1.26                | 0.83       |
| (1,3068) | 1:70:B:GLY:HA3  | 1:71:A:ILE:HG22 | 9                   | 1.52     | 1.26                | 0.83       |
| (1,3068) | 1:70:B:GLY:HA3  | 1:71:A:ILE:HG23 | 9                   | 1.52     | 1.26                | 0.83       |
| (1,3068) | 1:70:B:GLY:HA3  | 1:71:A:ILE:HG21 | 9                   | 1.52     | 1.26                | 0.83       |
| (1,2218) | 1:118:B:ARG:H   | 1:118:B:ARG:HG3 | 9                   | 1.4      | 0.36                | 1.38       |
| (1,2217) | 1:118:A:ARG:H   | 1:118:A:ARG:HG3 | 9                   | 1.39     | 0.36                | 1.36       |
| (1,1489) | 1:110:A:CYS:HB3 | 1:14:A:VAL:HG22 | 9                   | 0.93     | 1.14                | 0.65       |
| (1,1489) | 1:110:A:CYS:HB3 | 1:14:A:VAL:HG23 | 9                   | 0.93     | 1.14                | 0.65       |
| (1,1489) | 1:110:A:CYS:HB3 | 1:14:A:VAL:HG21 | 9                   | 0.93     | 1.14                | 0.65       |
| (1,1490) | 1:110:B:CYS:HB3 | 1:14:B:VAL:HG22 | 9                   | 0.93     | 1.14                | 0.65       |
| (1,1490) | 1:110:B:CYS:HB3 | 1:14:B:VAL:HG23 | 9                   | 0.93     | 1.14                | 0.65       |
| (1,1490) | 1:110:B:CYS:HB3 | 1:14:B:VAL:HG21 | 9                   | 0.93     | 1.14                | 0.65       |
| (1,1996) | 1:67:B:GLY:H    | 1:64:B:VAL:HB   | 9                   | 0.9      | 0.66                | 0.84       |
| (1,336)  | 1:36:B:VAL:HG13 | 1:30:B:ASP:HB2  | 9                   | 0.87     | 0.39                | 0.84       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,336)  | 1:36:B:VAL:HG11 | 1:30:B:ASP:HB2  | 9                   | 0.87     | 0.39                | 0.84       |
| (1,336)  | 1:36:B:VAL:HG12 | 1:30:B:ASP:HB2  | 9                   | 0.87     | 0.39                | 0.84       |
| (1,335)  | 1:36:A:VAL:HG13 | 1:30:A:ASP:HB2  | 9                   | 0.87     | 0.39                | 0.84       |
| (1,335)  | 1:36:A:VAL:HG11 | 1:30:A:ASP:HB2  | 9                   | 0.87     | 0.39                | 0.84       |
| (1,335)  | 1:36:A:VAL:HG12 | 1:30:A:ASP:HB2  | 9                   | 0.87     | 0.39                | 0.84       |
| (1,1313) | 1:70:A:GLY:H    | 1:64:A:VAL:HG13 | 9                   | 0.74     | 0.57                | 0.69       |
| (1,1313) | 1:70:A:GLY:H    | 1:64:A:VAL:HG12 | 9                   | 0.74     | 0.57                | 0.69       |
| (1,1313) | 1:70:A:GLY:H    | 1:64:A:VAL:HG11 | 9                   | 0.74     | 0.57                | 0.69       |
| (1,1314) | 1:70:B:GLY:H    | 1:64:B:VAL:HG13 | 9                   | 0.74     | 0.57                | 0.69       |
| (1,1314) | 1:70:B:GLY:H    | 1:64:B:VAL:HG12 | 9                   | 0.74     | 0.57                | 0.69       |
| (1,1314) | 1:70:B:GLY:H    | 1:64:B:VAL:HG11 | 9                   | 0.74     | 0.57                | 0.69       |
| (1,1170) | 1:39:B:LEU:HD11 | 1:92:B:MET:HG2  | 9                   | 0.72     | 0.77                | 0.29       |
| (1,1170) | 1:39:B:LEU:HD13 | 1:92:B:MET:HG2  | 9                   | 0.72     | 0.77                | 0.29       |
| (1,1169) | 1:39:A:LEU:HD11 | 1:92:A:MET:HG2  | 9                   | 0.72     | 0.77                | 0.28       |
| (1,1169) | 1:39:A:LEU:HD13 | 1:92:A:MET:HG2  | 9                   | 0.72     | 0.77                | 0.28       |
| (1,1391) | 1:59:A:ARG:HD2  | 1:18:A:VAL:HG12 | 9                   | 0.72     | 0.37                | 0.55       |
| (1,1391) | 1:59:A:ARG:HD2  | 1:18:A:VAL:HG13 | 9                   | 0.72     | 0.37                | 0.55       |
| (1,1391) | 1:59:A:ARG:HD2  | 1:18:A:VAL:HG11 | 9                   | 0.72     | 0.37                | 0.55       |
| (1,1392) | 1:59:B:ARG:HD2  | 1:18:B:VAL:HG12 | 9                   | 0.72     | 0.38                | 0.55       |
| (1,1392) | 1:59:B:ARG:HD2  | 1:18:B:VAL:HG13 | 9                   | 0.72     | 0.38                | 0.55       |
| (1,1392) | 1:59:B:ARG:HD2  | 1:18:B:VAL:HG11 | 9                   | 0.72     | 0.38                | 0.55       |
| (1,1610) | 1:24:B:ASP:H    | 1:22:B:VAL:HG22 | 9                   | 0.63     | 0.35                | 0.56       |
| (1,1610) | 1:24:B:ASP:H    | 1:22:B:VAL:HG23 | 9                   | 0.63     | 0.35                | 0.56       |
| (1,1610) | 1:24:B:ASP:H    | 1:22:B:VAL:HG21 | 9                   | 0.63     | 0.35                | 0.56       |
| (1,1609) | 1:24:A:ASP:H    | 1:22:A:VAL:HG22 | 9                   | 0.62     | 0.35                | 0.56       |
| (1,1609) | 1:24:A:ASP:H    | 1:22:A:VAL:HG23 | 9                   | 0.62     | 0.35                | 0.56       |
| (1,1609) | 1:24:A:ASP:H    | 1:22:A:VAL:HG21 | 9                   | 0.62     | 0.35                | 0.56       |
| (1,1450) | 1:25:B:LYS:HG2  | 1:53:B:PHE:HE1  | 9                   | 0.62     | 0.53                | 0.28       |
| (1,1449) | 1:25:A:LYS:HG2  | 1:53:A:PHE:HE1  | 9                   | 0.61     | 0.53                | 0.28       |
| (1,2769) | 1:18:A:VAL:H    | 1:57:A:LYS:HB2  | 9                   | 0.55     | 0.19                | 0.59       |
| (1,2770) | 1:18:B:VAL:H    | 1:57:B:LYS:HB2  | 9                   | 0.55     | 0.19                | 0.59       |
| (1,2701) | 1:104:A:ILE:H   | 1:103:A:ARG:HB3 | 9                   | 0.5      | 0.17                | 0.57       |
| (1,2702) | 1:104:B:ILE:H   | 1:103:B:ARG:HB3 | 9                   | 0.5      | 0.17                | 0.57       |
| (1,3034) | 1:35:B:GLU:H    | 1:34:B:LYS:HG3  | 9                   | 0.43     | 0.12                | 0.42       |
| (1,3033) | 1:35:A:GLU:H    | 1:34:A:LYS:HG3  | 9                   | 0.43     | 0.12                | 0.42       |
| (1,603)  | 1:104:A:ILE:HB  | 1:85:A:THR:HG22 | 9                   | 0.24     | 0.08                | 0.26       |
| (1,603)  | 1:104:A:ILE:HB  | 1:85:A:THR:HG23 | 9                   | 0.24     | 0.08                | 0.26       |
| (1,603)  | 1:104:A:ILE:HB  | 1:85:A:THR:HG21 | 9                   | 0.24     | 0.08                | 0.26       |
| (1,604)  | 1:104:B:ILE:HB  | 1:85:B:THR:HG22 | 9                   | 0.24     | 0.08                | 0.25       |
| (1,604)  | 1:104:B:ILE:HB  | 1:85:B:THR:HG23 | 9                   | 0.24     | 0.08                | 0.25       |
| (1,604)  | 1:104:B:ILE:HB  | 1:85:B:THR:HG21 | 9                   | 0.24     | 0.08                | 0.25       |
| (1,3073) | 1:114:A:ARG:H   | 1:12:B:PHE:HD2  | 8                   | 1.75     | 1.3                 | 1.75       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD1   | 8                   | 1.75     | 1.3                 | 1.75       |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD2   | 8                   | 1.73     | 1.3                 | 1.72       |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD1   | 8                   | 1.73     | 1.3                 | 1.72       |
| (1,3)    | 1:111:A:VAL:HG23 | 1:112:A:LEU:HD23 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,3)    | 1:111:A:VAL:HG22 | 1:112:A:LEU:HD22 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,3)    | 1:111:A:VAL:HG23 | 1:112:A:LEU:HD22 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,3)    | 1:111:A:VAL:HG22 | 1:112:A:LEU:HD23 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,3)    | 1:111:A:VAL:HG23 | 1:112:A:LEU:HD21 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,4)    | 1:111:B:VAL:HG23 | 1:112:B:LEU:HD23 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,4)    | 1:111:B:VAL:HG22 | 1:112:B:LEU:HD22 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,4)    | 1:111:B:VAL:HG23 | 1:112:B:LEU:HD22 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,4)    | 1:111:B:VAL:HG22 | 1:112:B:LEU:HD23 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,4)    | 1:111:B:VAL:HG23 | 1:112:B:LEU:HD21 | 8                   | 1.03     | 0.74                | 0.9        |
| (1,423)  | 1:87:A:VAL:HG12  | 1:53:A:PHE:HD1   | 8                   | 1.02     | 0.81                | 0.8        |
| (1,423)  | 1:87:A:VAL:HG11  | 1:53:A:PHE:HD1   | 8                   | 1.02     | 0.81                | 0.8        |
| (1,423)  | 1:87:A:VAL:HG13  | 1:53:A:PHE:HD1   | 8                   | 1.02     | 0.81                | 0.8        |
| (1,424)  | 1:87:B:VAL:HG12  | 1:53:B:PHE:HD1   | 8                   | 1.02     | 0.81                | 0.8        |
| (1,424)  | 1:87:B:VAL:HG11  | 1:53:B:PHE:HD1   | 8                   | 1.02     | 0.81                | 0.8        |
| (1,424)  | 1:87:B:VAL:HG13  | 1:53:B:PHE:HD1   | 8                   | 1.02     | 0.81                | 0.8        |
| (1,1995) | 1:67:A:GLY:H     | 1:64:A:VAL:HB    | 8                   | 1.0      | 0.64                | 0.89       |
| (1,1420) | 1:6:B:ILE:HG12   | 1:6:B:ILE:HG21   | 8                   | 0.97     | 0.5                 | 1.26       |
| (1,1420) | 1:6:B:ILE:HG12   | 1:6:B:ILE:HG23   | 8                   | 0.97     | 0.5                 | 1.26       |
| (1,1420) | 1:6:B:ILE:HG12   | 1:6:B:ILE:HG22   | 8                   | 0.97     | 0.5                 | 1.26       |
| (1,1419) | 1:6:A:ILE:HG12   | 1:6:A:ILE:HG21   | 8                   | 0.97     | 0.5                 | 1.26       |
| (1,1419) | 1:6:A:ILE:HG12   | 1:6:A:ILE:HG23   | 8                   | 0.97     | 0.5                 | 1.26       |
| (1,1419) | 1:6:A:ILE:HG12   | 1:6:A:ILE:HG22   | 8                   | 0.97     | 0.5                 | 1.26       |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD12  | 8                   | 0.83     | 0.71                | 0.57       |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD11  | 8                   | 0.83     | 0.71                | 0.57       |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD13  | 8                   | 0.83     | 0.71                | 0.57       |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD12  | 8                   | 0.81     | 0.71                | 0.54       |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD11  | 8                   | 0.81     | 0.71                | 0.54       |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD13  | 8                   | 0.81     | 0.71                | 0.54       |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG11 | 8                   | 0.8      | 0.52                | 0.78       |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG13 | 8                   | 0.8      | 0.52                | 0.78       |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG11 | 8                   | 0.8      | 0.52                | 0.78       |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG13 | 8                   | 0.8      | 0.52                | 0.78       |
| (1,1445) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HG2   | 8                   | 0.46     | 0.07                | 0.46       |
| (1,1446) | 1:25:B:LYS:HE3   | 1:25:B:LYS:HG2   | 8                   | 0.45     | 0.07                | 0.46       |
| (1,257)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HB2   | 8                   | 0.43     | 0.26                | 0.38       |
| (1,257)  | 1:112:A:LEU:HD21 | 1:76:A:TRP:HB2   | 8                   | 0.43     | 0.26                | 0.38       |
| (1,258)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HB2   | 8                   | 0.43     | 0.26                | 0.38       |
| (1,258)  | 1:112:B:LEU:HD21 | 1:76:B:TRP:HB2   | 8                   | 0.43     | 0.26                | 0.38       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,157)  | 1:40:A:GLY:HA2  | 1:41:A:GLU:HG2   | 8                   | 0.4      | 0.06                | 0.42       |
| (1,158)  | 1:40:B:GLY:HA2  | 1:41:B:GLU:HG2   | 8                   | 0.4      | 0.06                | 0.42       |
| (1,565)  | 1:57:A:LYS:HD2  | 1:57:A:LYS:HG2   | 8                   | 0.36     | 0.0                 | 0.36       |
| (1,566)  | 1:57:B:LYS:HD2  | 1:57:B:LYS:HG2   | 8                   | 0.36     | 0.0                 | 0.36       |
| (1,297)  | 1:118:A:ARG:HB3 | 1:118:A:ARG:HG2  | 8                   | 0.32     | 0.0                 | 0.32       |
| (1,298)  | 1:118:B:ARG:HB3 | 1:118:B:ARG:HG2  | 8                   | 0.32     | 0.0                 | 0.32       |
| (1,3091) | 1:86:A:PHE:H    | 1:54:B:PHE:HD1   | 8                   | 0.27     | 0.14                | 0.21       |
| (1,3091) | 1:86:A:PHE:H    | 1:54:B:PHE:HD2   | 8                   | 0.27     | 0.14                | 0.21       |
| (1,3092) | 1:86:B:PHE:H    | 1:54:A:PHE:HD1   | 8                   | 0.27     | 0.16                | 0.2        |
| (1,3092) | 1:86:B:PHE:H    | 1:54:A:PHE:HD2   | 8                   | 0.27     | 0.16                | 0.2        |
| (1,1649) | 1:47:A:SER:H    | 1:48:A:VAL:HG12  | 8                   | 0.26     | 0.13                | 0.24       |
| (1,1649) | 1:47:A:SER:H    | 1:48:A:VAL:HG11  | 8                   | 0.26     | 0.13                | 0.24       |
| (1,1650) | 1:47:B:SER:H    | 1:48:B:VAL:HG12  | 8                   | 0.26     | 0.13                | 0.24       |
| (1,1650) | 1:47:B:SER:H    | 1:48:B:VAL:HG11  | 8                   | 0.26     | 0.13                | 0.24       |
| (1,281)  | 1:37:A:MET:HA   | 1:37:A:MET:HE3   | 8                   | 0.24     | 0.1                 | 0.22       |
| (1,281)  | 1:37:A:MET:HA   | 1:37:A:MET:HE1   | 8                   | 0.24     | 0.1                 | 0.22       |
| (1,281)  | 1:37:A:MET:HA   | 1:37:A:MET:HE2   | 8                   | 0.24     | 0.1                 | 0.22       |
| (1,2013) | 1:79:A:TYR:H    | 1:111:A:VAL:HB   | 8                   | 0.22     | 0.11                | 0.18       |
| (1,2014) | 1:79:B:TYR:H    | 1:111:B:VAL:HB   | 8                   | 0.22     | 0.11                | 0.18       |
| (1,1880) | 1:21:B:TRP:H    | 1:20:B:VAL:HG21  | 8                   | 0.21     | 0.09                | 0.19       |
| (1,1880) | 1:21:B:TRP:H    | 1:20:B:VAL:HG23  | 8                   | 0.21     | 0.09                | 0.19       |
| (1,1880) | 1:21:B:TRP:H    | 1:20:B:VAL:HG22  | 8                   | 0.21     | 0.09                | 0.19       |
| (1,1879) | 1:21:A:TRP:H    | 1:20:A:VAL:HG21  | 8                   | 0.21     | 0.09                | 0.18       |
| (1,1879) | 1:21:A:TRP:H    | 1:20:A:VAL:HG23  | 8                   | 0.21     | 0.09                | 0.18       |
| (1,1879) | 1:21:A:TRP:H    | 1:20:A:VAL:HG22  | 8                   | 0.21     | 0.09                | 0.18       |
| (1,417)  | 1:38:A:VAL:HG13 | 1:38:A:VAL:HB    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,417)  | 1:38:A:VAL:HG11 | 1:38:A:VAL:HB    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,417)  | 1:38:A:VAL:HG12 | 1:38:A:VAL:HB    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,418)  | 1:38:B:VAL:HG13 | 1:38:B:VAL:HB    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,418)  | 1:38:B:VAL:HG11 | 1:38:B:VAL:HB    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,418)  | 1:38:B:VAL:HG12 | 1:38:B:VAL:HB    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,356)  | 1:41:B:GLU:HG2  | 1:48:B:VAL:HA    | 7                   | 1.58     | 0.59                | 1.56       |
| (1,355)  | 1:41:A:GLU:HG2  | 1:48:A:VAL:HA    | 7                   | 1.57     | 0.59                | 1.55       |
| (1,426)  | 1:87:B:VAL:HG12 | 1:53:B:PHE:HE1   | 7                   | 1.29     | 0.85                | 1.49       |
| (1,426)  | 1:87:B:VAL:HG11 | 1:53:B:PHE:HE1   | 7                   | 1.29     | 0.85                | 1.49       |
| (1,426)  | 1:87:B:VAL:HG13 | 1:53:B:PHE:HE1   | 7                   | 1.29     | 0.85                | 1.49       |
| (1,425)  | 1:87:A:VAL:HG12 | 1:53:A:PHE:HE1   | 7                   | 1.29     | 0.85                | 1.49       |
| (1,425)  | 1:87:A:VAL:HG11 | 1:53:A:PHE:HE1   | 7                   | 1.29     | 0.85                | 1.49       |
| (1,425)  | 1:87:A:VAL:HG13 | 1:53:A:PHE:HE1   | 7                   | 1.29     | 0.85                | 1.49       |
| (1,3080) | 1:11:B:GLU:HG2  | 1:111:A:VAL:HG23 | 7                   | 1.18     | 0.78                | 1.23       |
| (1,3080) | 1:11:B:GLU:HG2  | 1:111:A:VAL:HG21 | 7                   | 1.18     | 0.78                | 1.23       |
| (1,3080) | 1:11:B:GLU:HG2  | 1:111:A:VAL:HG22 | 7                   | 1.18     | 0.78                | 1.23       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG23 | 7                   | 1.17     | 0.79                | 1.23       |
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG21 | 7                   | 1.17     | 0.79                | 1.23       |
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG22 | 7                   | 1.17     | 0.79                | 1.23       |
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 7                   | 1.16     | 0.13                | 1.15       |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 7                   | 1.16     | 0.14                | 1.15       |
| (1,3085) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HG23  | 7                   | 0.87     | 0.49                | 0.73       |
| (1,3085) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HG22  | 7                   | 0.87     | 0.49                | 0.73       |
| (1,3085) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HG23  | 7                   | 0.87     | 0.49                | 0.73       |
| (1,3085) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HG21  | 7                   | 0.87     | 0.49                | 0.73       |
| (1,3085) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HG23  | 7                   | 0.87     | 0.49                | 0.73       |
| (1,3085) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HG21  | 7                   | 0.87     | 0.49                | 0.73       |
| (1,3086) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HG23  | 7                   | 0.85     | 0.49                | 0.71       |
| (1,3086) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HG22  | 7                   | 0.85     | 0.49                | 0.71       |
| (1,3086) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HG23  | 7                   | 0.85     | 0.49                | 0.71       |
| (1,3086) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HG21  | 7                   | 0.85     | 0.49                | 0.71       |
| (1,3086) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HG23  | 7                   | 0.85     | 0.49                | 0.71       |
| (1,3086) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HG21  | 7                   | 0.85     | 0.49                | 0.71       |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 7                   | 0.45     | 0.2                 | 0.39       |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 7                   | 0.45     | 0.2                 | 0.39       |
| (1,1872) | 1:21:B:TRP:HE1   | 1:21:B:TRP:H     | 7                   | 0.42     | 0.1                 | 0.39       |
| (1,1871) | 1:21:A:TRP:HE1   | 1:21:A:TRP:H     | 7                   | 0.42     | 0.1                 | 0.4        |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE1   | 7                   | 0.26     | 0.09                | 0.26       |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE3   | 7                   | 0.26     | 0.09                | 0.26       |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE2   | 7                   | 0.26     | 0.09                | 0.26       |
| (1,2720) | 1:84:B:HIS:H     | 1:83:B:THR:HB    | 7                   | 0.19     | 0.06                | 0.17       |
| (1,2719) | 1:84:A:HIS:H     | 1:83:A:THR:HB    | 7                   | 0.18     | 0.06                | 0.17       |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG12 | 7                   | 0.11     | 0.01                | 0.1        |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG13 | 7                   | 0.11     | 0.01                | 0.1        |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG11 | 7                   | 0.11     | 0.01                | 0.1        |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG12 | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG13 | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG11 | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,2255) | 1:77:A:ASN:HD22  | 1:115:A:LYS:HG2  | 6                   | 1.44     | 1.71                | 0.7        |
| (1,2256) | 1:77:B:ASN:HD22  | 1:115:B:LYS:HG2  | 6                   | 1.43     | 1.7                 | 0.7        |
| (1,2501) | 1:69:A:ARG:H     | 1:64:A:VAL:HG11  | 6                   | 1.1      | 0.5                 | 1.06       |
| (1,2501) | 1:69:A:ARG:H     | 1:64:A:VAL:HG12  | 6                   | 1.1      | 0.5                 | 1.06       |
| (1,2501) | 1:69:A:ARG:H     | 1:64:A:VAL:HG13  | 6                   | 1.1      | 0.5                 | 1.06       |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG11  | 6                   | 1.1      | 0.5                 | 1.06       |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG12  | 6                   | 1.1      | 0.5                 | 1.06       |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG13  | 6                   | 1.1      | 0.5                 | 1.06       |
| (1,953)  | 1:18:A:VAL:HG23  | 1:59:A:ARG:HD2   | 6                   | 1.04     | 0.52                | 1.08       |
| (1,953)  | 1:18:A:VAL:HG21  | 1:59:A:ARG:HD2   | 6                   | 1.04     | 0.52                | 1.08       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,953)  | 1:18:A:VAL:HG22 | 1:59:A:ARG:HD2   | 6                   | 1.04     | 0.52                | 1.08       |
| (1,954)  | 1:18:B:VAL:HG23 | 1:59:B:ARG:HD2   | 6                   | 1.04     | 0.52                | 1.08       |
| (1,954)  | 1:18:B:VAL:HG21 | 1:59:B:ARG:HD2   | 6                   | 1.04     | 0.52                | 1.08       |
| (1,954)  | 1:18:B:VAL:HG22 | 1:59:B:ARG:HD2   | 6                   | 1.04     | 0.52                | 1.08       |
| (1,2608) | 1:107:B:ALA:H   | 1:56:B:THR:HG22  | 6                   | 0.96     | 0.51                | 0.96       |
| (1,2608) | 1:107:B:ALA:H   | 1:56:B:THR:HG21  | 6                   | 0.96     | 0.51                | 0.96       |
| (1,2608) | 1:107:B:ALA:H   | 1:56:B:THR:HG23  | 6                   | 0.96     | 0.51                | 0.96       |
| (1,2607) | 1:107:A:ALA:H   | 1:56:A:THR:HG22  | 6                   | 0.96     | 0.51                | 0.96       |
| (1,2607) | 1:107:A:ALA:H   | 1:56:A:THR:HG21  | 6                   | 0.96     | 0.51                | 0.96       |
| (1,2607) | 1:107:A:ALA:H   | 1:56:A:THR:HG23  | 6                   | 0.96     | 0.51                | 0.96       |
| (1,1544) | 1:55:B:GLU:HG3  | 1:20:B:VAL:HG22  | 6                   | 0.93     | 0.3                 | 0.78       |
| (1,1544) | 1:55:B:GLU:HG3  | 1:20:B:VAL:HG23  | 6                   | 0.93     | 0.3                 | 0.78       |
| (1,1544) | 1:55:B:GLU:HG3  | 1:20:B:VAL:HG21  | 6                   | 0.93     | 0.3                 | 0.78       |
| (1,1543) | 1:55:A:GLU:HG3  | 1:20:A:VAL:HG22  | 6                   | 0.93     | 0.3                 | 0.76       |
| (1,1543) | 1:55:A:GLU:HG3  | 1:20:A:VAL:HG23  | 6                   | 0.93     | 0.3                 | 0.76       |
| (1,1543) | 1:55:A:GLU:HG3  | 1:20:A:VAL:HG21  | 6                   | 0.93     | 0.3                 | 0.76       |
| (1,3082) | 1:12:B:PHE:H    | 1:111:A:VAL:HG22 | 6                   | 0.8      | 0.22                | 0.87       |
| (1,3082) | 1:12:B:PHE:H    | 1:111:A:VAL:HG21 | 6                   | 0.8      | 0.22                | 0.87       |
| (1,3081) | 1:12:A:PHE:H    | 1:111:B:VAL:HG22 | 6                   | 0.79     | 0.24                | 0.85       |
| (1,3081) | 1:12:A:PHE:H    | 1:111:B:VAL:HG21 | 6                   | 0.79     | 0.24                | 0.85       |
| (1,1909) | 1:72:A:ASP:H    | 1:71:A:ILE:HG21  | 6                   | 0.75     | 0.44                | 0.81       |
| (1,1909) | 1:72:A:ASP:H    | 1:71:A:ILE:HG23  | 6                   | 0.75     | 0.44                | 0.81       |
| (1,1909) | 1:72:A:ASP:H    | 1:71:A:ILE:HG22  | 6                   | 0.75     | 0.44                | 0.81       |
| (1,1910) | 1:72:B:ASP:H    | 1:71:B:ILE:HG21  | 6                   | 0.75     | 0.44                | 0.8        |
| (1,1910) | 1:72:B:ASP:H    | 1:71:B:ILE:HG23  | 6                   | 0.75     | 0.44                | 0.8        |
| (1,1910) | 1:72:B:ASP:H    | 1:71:B:ILE:HG22  | 6                   | 0.75     | 0.44                | 0.8        |
| (1,743)  | 1:47:A:SER:HB2  | 1:47:A:SER:HA    | 6                   | 0.54     | 0.0                 | 0.54       |
| (1,744)  | 1:47:B:SER:HB2  | 1:47:B:SER:HA    | 6                   | 0.54     | 0.0                 | 0.54       |
| (1,2151) | 1:77:A:ASN:H    | 1:115:A:LYS:HD2  | 6                   | 0.47     | 0.21                | 0.42       |
| (1,2152) | 1:77:B:ASN:H    | 1:115:B:LYS:HD2  | 6                   | 0.47     | 0.21                | 0.42       |
| (1,2083) | 1:88:A:LYS:H    | 1:88:A:LYS:HD2   | 6                   | 0.42     | 0.28                | 0.36       |
| (1,2084) | 1:88:B:LYS:H    | 1:88:B:LYS:HD2   | 6                   | 0.42     | 0.27                | 0.35       |
| (1,1384) | 1:18:B:VAL:HG23 | 1:59:B:ARG:HG2   | 6                   | 0.4      | 0.15                | 0.42       |
| (1,1384) | 1:18:B:VAL:HG21 | 1:59:B:ARG:HG2   | 6                   | 0.4      | 0.15                | 0.42       |
| (1,1384) | 1:18:B:VAL:HG22 | 1:59:B:ARG:HG2   | 6                   | 0.4      | 0.15                | 0.42       |
| (1,1383) | 1:18:A:VAL:HG23 | 1:59:A:ARG:HG2   | 6                   | 0.39     | 0.15                | 0.42       |
| (1,1383) | 1:18:A:VAL:HG21 | 1:59:A:ARG:HG2   | 6                   | 0.39     | 0.15                | 0.42       |
| (1,1383) | 1:18:A:VAL:HG22 | 1:59:A:ARG:HG2   | 6                   | 0.39     | 0.15                | 0.42       |
| (1,1659) | 1:47:A:SER:H    | 1:47:A:SER:HB3   | 6                   | 0.36     | 0.01                | 0.36       |
| (1,1660) | 1:47:B:SER:H    | 1:47:B:SER:HB3   | 6                   | 0.36     | 0.01                | 0.36       |
| (1,2195) | 1:55:A:GLU:H    | 1:22:A:VAL:HG11  | 6                   | 0.36     | 0.16                | 0.33       |
| (1,2195) | 1:55:A:GLU:H    | 1:22:A:VAL:HG12  | 6                   | 0.36     | 0.16                | 0.33       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2196) | 1:55:B:GLU:H     | 1:22:B:VAL:HG11 | 6                   | 0.36     | 0.15                | 0.33       |
| (1,2196) | 1:55:B:GLU:H     | 1:22:B:VAL:HG12 | 6                   | 0.36     | 0.15                | 0.33       |
| (1,1297) | 1:36:A:VAL:HG21  | 1:91:A:THR:H    | 6                   | 0.32     | 0.14                | 0.3        |
| (1,1297) | 1:36:A:VAL:HG23  | 1:91:A:THR:H    | 6                   | 0.32     | 0.14                | 0.3        |
| (1,1297) | 1:36:A:VAL:HG22  | 1:91:A:THR:H    | 6                   | 0.32     | 0.14                | 0.3        |
| (1,1298) | 1:36:B:VAL:HG21  | 1:91:B:THR:H    | 6                   | 0.32     | 0.14                | 0.3        |
| (1,1298) | 1:36:B:VAL:HG23  | 1:91:B:THR:H    | 6                   | 0.32     | 0.14                | 0.3        |
| (1,1298) | 1:36:B:VAL:HG22  | 1:91:B:THR:H    | 6                   | 0.32     | 0.14                | 0.3        |
| (1,2107) | 1:117:A:VAL:H    | 1:117:A:VAL:HB  | 6                   | 0.24     | 0.02                | 0.24       |
| (1,2108) | 1:117:B:VAL:H    | 1:117:B:VAL:HB  | 6                   | 0.24     | 0.02                | 0.24       |
| (1,1898) | 1:48:B:VAL:H     | 1:48:B:VAL:HG12 | 6                   | 0.22     | 0.18                | 0.15       |
| (1,1898) | 1:48:B:VAL:H     | 1:48:B:VAL:HG13 | 6                   | 0.22     | 0.18                | 0.15       |
| (1,1898) | 1:48:B:VAL:H     | 1:48:B:VAL:HG11 | 6                   | 0.22     | 0.18                | 0.15       |
| (1,1361) | 1:104:A:ILE:HB   | 1:87:A:VAL:HG21 | 6                   | 0.16     | 0.06                | 0.14       |
| (1,1361) | 1:104:A:ILE:HB   | 1:87:A:VAL:HG22 | 6                   | 0.16     | 0.06                | 0.14       |
| (1,1362) | 1:104:B:ILE:HB   | 1:87:B:VAL:HG21 | 6                   | 0.16     | 0.06                | 0.14       |
| (1,1362) | 1:104:B:ILE:HB   | 1:87:B:VAL:HG22 | 6                   | 0.16     | 0.06                | 0.14       |
| (1,2503) | 1:30:A:ASP:H     | 1:34:A:LYS:HB2  | 6                   | 0.15     | 0.02                | 0.16       |
| (1,2504) | 1:30:B:ASP:H     | 1:34:B:LYS:HB2  | 6                   | 0.15     | 0.02                | 0.16       |
| (1,2545) | 1:72:A:ASP:H     | 1:76:A:TRP:HE1  | 5                   | 1.54     | 1.28                | 1.06       |
| (1,2546) | 1:72:B:ASP:H     | 1:76:B:TRP:HE1  | 5                   | 1.53     | 1.29                | 1.05       |
| (1,1886) | 1:21:B:TRP:H     | 1:54:B:PHE:HD1  | 5                   | 1.52     | 0.3                 | 1.59       |
| (1,1885) | 1:21:A:TRP:H     | 1:54:A:PHE:HD1  | 5                   | 1.51     | 0.3                 | 1.58       |
| (1,2160) | 1:77:B:ASN:H     | 1:115:B:LYS:HG2 | 5                   | 0.79     | 0.35                | 0.83       |
| (1,2159) | 1:77:A:ASN:H     | 1:115:A:LYS:HG2 | 5                   | 0.79     | 0.35                | 0.82       |
| (1,3052) | 1:21:B:TRP:HE1   | 1:31:A:ILE:HD13 | 5                   | 0.79     | 0.36                | 0.73       |
| (1,3052) | 1:21:B:TRP:HE1   | 1:31:A:ILE:HD12 | 5                   | 0.79     | 0.36                | 0.73       |
| (1,3051) | 1:21:A:TRP:HE1   | 1:31:B:ILE:HD13 | 5                   | 0.78     | 0.35                | 0.72       |
| (1,3051) | 1:21:A:TRP:HE1   | 1:31:B:ILE:HD12 | 5                   | 0.78     | 0.35                | 0.72       |
| (1,1331) | 1:64:A:VAL:HG21  | 1:65:A:ASP:HB3  | 5                   | 0.61     | 0.54                | 0.23       |
| (1,1331) | 1:64:A:VAL:HG23  | 1:65:A:ASP:HB3  | 5                   | 0.61     | 0.54                | 0.23       |
| (1,1331) | 1:64:A:VAL:HG22  | 1:65:A:ASP:HB3  | 5                   | 0.61     | 0.54                | 0.23       |
| (1,1332) | 1:64:B:VAL:HG21  | 1:65:B:ASP:HB3  | 5                   | 0.61     | 0.54                | 0.22       |
| (1,1332) | 1:64:B:VAL:HG23  | 1:65:B:ASP:HB3  | 5                   | 0.61     | 0.54                | 0.22       |
| (1,1332) | 1:64:B:VAL:HG22  | 1:65:B:ASP:HB3  | 5                   | 0.61     | 0.54                | 0.22       |
| (1,676)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HE2  | 5                   | 0.52     | 0.03                | 0.52       |
| (1,675)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HE2  | 5                   | 0.52     | 0.03                | 0.52       |
| (1,71)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG2  | 5                   | 0.43     | 0.22                | 0.33       |
| (1,72)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG2  | 5                   | 0.43     | 0.22                | 0.33       |
| (1,553)  | 1:88:A:LYS:HG2   | 1:88:A:LYS:HE2  | 5                   | 0.4      | 0.11                | 0.45       |
| (1,554)  | 1:88:B:LYS:HG2   | 1:88:B:LYS:HE2  | 5                   | 0.4      | 0.11                | 0.44       |
| (1,402)  | 1:102:B:ILE:HD12 | 1:25:B:LYS:HG2  | 5                   | 0.38     | 0.24                | 0.28       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,402)  | 1:102:B:ILE:HD11 | 1:25:B:LYS:HG2   | 5                   | 0.38     | 0.24                | 0.28       |
| (1,402)  | 1:102:B:ILE:HD13 | 1:25:B:LYS:HG2   | 5                   | 0.38     | 0.24                | 0.28       |
| (1,401)  | 1:102:A:ILE:HD12 | 1:25:A:LYS:HG2   | 5                   | 0.38     | 0.24                | 0.28       |
| (1,401)  | 1:102:A:ILE:HD11 | 1:25:A:LYS:HG2   | 5                   | 0.38     | 0.24                | 0.28       |
| (1,401)  | 1:102:A:ILE:HD13 | 1:25:A:LYS:HG2   | 5                   | 0.38     | 0.24                | 0.28       |
| (1,3094) | 1:86:B:PHE:H     | 1:54:A:PHE:HE1   | 5                   | 0.33     | 0.2                 | 0.34       |
| (1,3094) | 1:86:B:PHE:H     | 1:54:A:PHE:HE2   | 5                   | 0.33     | 0.2                 | 0.34       |
| (1,2031) | 1:27:A:THR:H     | 1:38:A:VAL:HG23  | 5                   | 0.31     | 0.16                | 0.34       |
| (1,2031) | 1:27:A:THR:H     | 1:38:A:VAL:HG21  | 5                   | 0.31     | 0.16                | 0.34       |
| (1,2031) | 1:27:A:THR:H     | 1:38:A:VAL:HG22  | 5                   | 0.31     | 0.16                | 0.34       |
| (1,2032) | 1:27:B:THR:H     | 1:38:B:VAL:HG23  | 5                   | 0.31     | 0.15                | 0.34       |
| (1,2032) | 1:27:B:THR:H     | 1:38:B:VAL:HG21  | 5                   | 0.31     | 0.15                | 0.34       |
| (1,2032) | 1:27:B:THR:H     | 1:38:B:VAL:HG22  | 5                   | 0.31     | 0.15                | 0.34       |
| (1,1897) | 1:48:A:VAL:H     | 1:48:A:VAL:HG12  | 5                   | 0.24     | 0.2                 | 0.16       |
| (1,1897) | 1:48:A:VAL:H     | 1:48:A:VAL:HG13  | 5                   | 0.24     | 0.2                 | 0.16       |
| (1,1897) | 1:48:A:VAL:H     | 1:48:A:VAL:HG11  | 5                   | 0.24     | 0.2                 | 0.16       |
| (1,2560) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD13 | 4                   | 2.02     | 1.11                | 2.34       |
| (1,2560) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD12 | 4                   | 2.02     | 1.11                | 2.34       |
| (1,2559) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD13 | 4                   | 2.02     | 1.1                 | 2.34       |
| (1,2559) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD12 | 4                   | 2.02     | 1.1                 | 2.34       |
| (3,1)    | 1:52:A:TYR:HB2   | 1:51:A:GLN:HG3   | 4                   | 1.38     | 0.24                | 1.42       |
| (3,1)    | 1:52:A:TYR:HB2   | 1:22:A:VAL:HB    | 4                   | 1.38     | 0.24                | 1.42       |
| (3,2)    | 1:52:B:TYR:HB2   | 1:51:B:GLN:HG3   | 4                   | 1.38     | 0.24                | 1.42       |
| (3,2)    | 1:52:B:TYR:HB2   | 1:22:B:VAL:HB    | 4                   | 1.38     | 0.24                | 1.42       |
| (1,1130) | 1:77:B:ASN:HB2   | 1:113:B:SER:HB2  | 4                   | 1.24     | 0.08                | 1.25       |
| (1,1129) | 1:77:A:ASN:HB2   | 1:113:A:SER:HB2  | 4                   | 1.23     | 0.08                | 1.25       |
| (1,818)  | 1:31:B:ILE:HG23  | 1:32:B:LYS:HG2   | 4                   | 1.05     | 0.09                | 1.08       |
| (1,818)  | 1:31:B:ILE:HG22  | 1:32:B:LYS:HG2   | 4                   | 1.05     | 0.09                | 1.08       |
| (1,818)  | 1:31:B:ILE:HG21  | 1:32:B:LYS:HG2   | 4                   | 1.05     | 0.09                | 1.08       |
| (1,817)  | 1:31:A:ILE:HG23  | 1:32:A:LYS:HG2   | 4                   | 1.04     | 0.08                | 1.07       |
| (1,817)  | 1:31:A:ILE:HG22  | 1:32:A:LYS:HG2   | 4                   | 1.04     | 0.08                | 1.07       |
| (1,817)  | 1:31:A:ILE:HG21  | 1:32:A:LYS:HG2   | 4                   | 1.04     | 0.08                | 1.07       |
| (1,3090) | 1:112:B:LEU:HD22 | 1:14:A:VAL:HA    | 4                   | 1.04     | 0.9                 | 0.64       |
| (1,3090) | 1:112:B:LEU:HD21 | 1:14:A:VAL:HA    | 4                   | 1.04     | 0.9                 | 0.64       |
| (1,3089) | 1:112:A:LEU:HD22 | 1:14:B:VAL:HA    | 4                   | 1.03     | 0.92                | 0.6        |
| (1,3089) | 1:112:A:LEU:HD21 | 1:14:B:VAL:HA    | 4                   | 1.03     | 0.92                | 0.6        |
| (1,1475) | 1:112:A:LEU:HD11 | 1:71:A:ILE:HA    | 4                   | 0.73     | 0.4                 | 0.62       |
| (1,1475) | 1:112:A:LEU:HD13 | 1:71:A:ILE:HA    | 4                   | 0.73     | 0.4                 | 0.62       |
| (1,1475) | 1:112:A:LEU:HD12 | 1:71:A:ILE:HA    | 4                   | 0.73     | 0.4                 | 0.62       |
| (1,1476) | 1:112:B:LEU:HD11 | 1:71:B:ILE:HA    | 4                   | 0.73     | 0.4                 | 0.62       |
| (1,1476) | 1:112:B:LEU:HD13 | 1:71:B:ILE:HA    | 4                   | 0.73     | 0.4                 | 0.62       |
| (1,1476) | 1:112:B:LEU:HD12 | 1:71:B:ILE:HA    | 4                   | 0.73     | 0.4                 | 0.62       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2555) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HB2  | 4                   | 0.66     | 0.34                | 0.6        |
| (1,2556) | 1:76:B:TRP:HE1  | 1:112:B:LEU:HB2  | 4                   | 0.66     | 0.34                | 0.6        |
| (1,3072) | 1:44:B:ILE:HD13 | 1:99:A:TRP:HE1   | 4                   | 0.58     | 0.32                | 0.54       |
| (1,3072) | 1:44:B:ILE:HD11 | 1:99:A:TRP:HE1   | 4                   | 0.58     | 0.32                | 0.54       |
| (1,3071) | 1:44:A:ILE:HD13 | 1:99:B:TRP:HE1   | 4                   | 0.58     | 0.33                | 0.55       |
| (1,3071) | 1:44:A:ILE:HD11 | 1:99:B:TRP:HE1   | 4                   | 0.58     | 0.33                | 0.55       |
| (1,2735) | 1:51:A:GLN:HE21 | 1:90:A:LEU:H     | 4                   | 0.56     | 0.26                | 0.59       |
| (1,2736) | 1:51:B:GLN:HE21 | 1:90:B:LEU:H     | 4                   | 0.55     | 0.25                | 0.59       |
| (1,2141) | 1:32:A:LYS:H    | 1:32:A:LYS:HG2   | 4                   | 0.55     | 0.07                | 0.58       |
| (1,2142) | 1:32:B:LYS:H    | 1:32:B:LYS:HG2   | 4                   | 0.55     | 0.07                | 0.58       |
| (1,2603) | 1:107:A:ALA:H   | 1:82:A:THR:HA    | 4                   | 0.44     | 0.12                | 0.48       |
| (1,2604) | 1:107:B:ALA:H   | 1:82:B:THR:HA    | 4                   | 0.43     | 0.12                | 0.48       |
| (1,3093) | 1:86:A:PHE:H    | 1:54:B:PHE:HE2   | 4                   | 0.38     | 0.18                | 0.39       |
| (1,3093) | 1:86:A:PHE:H    | 1:54:B:PHE:HE1   | 4                   | 0.38     | 0.18                | 0.39       |
| (1,2001) | 1:79:A:TYR:H    | 1:111:A:VAL:HA   | 4                   | 0.34     | 0.1                 | 0.36       |
| (1,2002) | 1:79:B:TYR:H    | 1:111:B:VAL:HA   | 4                   | 0.33     | 0.1                 | 0.35       |
| (1,809)  | 1:118:A:ARG:HB2 | 1:118:A:ARG:HG2  | 4                   | 0.27     | 0.16                | 0.24       |
| (1,810)  | 1:118:B:ARG:HB2 | 1:118:B:ARG:HG2  | 4                   | 0.27     | 0.16                | 0.24       |
| (1,1187) | 1:31:A:ILE:HD13 | 1:101:A:PHE:HB2  | 4                   | 0.26     | 0.06                | 0.26       |
| (1,1187) | 1:31:A:ILE:HD12 | 1:101:A:PHE:HB2  | 4                   | 0.26     | 0.06                | 0.26       |
| (1,1187) | 1:31:A:ILE:HD11 | 1:101:A:PHE:HB2  | 4                   | 0.26     | 0.06                | 0.26       |
| (1,1188) | 1:31:B:ILE:HD13 | 1:101:B:PHE:HB2  | 4                   | 0.25     | 0.07                | 0.25       |
| (1,1188) | 1:31:B:ILE:HD12 | 1:101:B:PHE:HB2  | 4                   | 0.25     | 0.07                | 0.25       |
| (1,1188) | 1:31:B:ILE:HD11 | 1:101:B:PHE:HB2  | 4                   | 0.25     | 0.07                | 0.25       |
| (1,874)  | 1:39:B:LEU:HD12 | 1:91:B:THR:HA    | 4                   | 0.23     | 0.09                | 0.24       |
| (1,874)  | 1:39:B:LEU:HD13 | 1:91:B:THR:HA    | 4                   | 0.23     | 0.09                | 0.24       |
| (1,2112) | 1:117:B:VAL:H   | 1:116:B:ALA:HB2  | 4                   | 0.22     | 0.18                | 0.12       |
| (1,2112) | 1:117:B:VAL:H   | 1:116:B:ALA:HB1  | 4                   | 0.22     | 0.18                | 0.12       |
| (1,2111) | 1:117:A:VAL:H   | 1:116:A:ALA:HB2  | 4                   | 0.22     | 0.18                | 0.12       |
| (1,2111) | 1:117:A:VAL:H   | 1:116:A:ALA:HB1  | 4                   | 0.22     | 0.18                | 0.12       |
| (1,279)  | 1:88:A:LYS:HB2  | 1:88:A:LYS:HD2   | 4                   | 0.2      | 0.05                | 0.22       |
| (1,280)  | 1:88:B:LYS:HB2  | 1:88:B:LYS:HD2   | 4                   | 0.2      | 0.05                | 0.22       |
| (1,2125) | 1:32:A:LYS:H    | 1:31:A:ILE:HG12  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,2126) | 1:32:B:LYS:H    | 1:31:B:ILE:HG12  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,600)  | 1:107:B:ALA:HB1 | 1:107:B:ALA:HA   | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,600)  | 1:107:B:ALA:HB2 | 1:107:B:ALA:HA   | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,599)  | 1:107:A:ALA:HB1 | 1:107:A:ALA:HA   | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,599)  | 1:107:A:ALA:HB2 | 1:107:A:ALA:HA   | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,3061) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HD13 | 3                   | 2.45     | 1.36                | 2.04       |
| (1,3061) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HD12 | 3                   | 2.45     | 1.36                | 2.04       |
| (1,3062) | 1:70:B:GLY:HA3  | 1:112:A:LEU:HD13 | 3                   | 2.43     | 1.36                | 2.02       |
| (1,3062) | 1:70:B:GLY:HA3  | 1:112:A:LEU:HD12 | 3                   | 2.43     | 1.36                | 2.02       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,138)  | 1:39:B:LEU:HG   | 1:92:B:MET:HG2  | 3                   | 1.67     | 0.17                | 1.56       |
| (1,137)  | 1:39:A:LEU:HG   | 1:92:A:MET:HG2  | 3                   | 1.67     | 0.18                | 1.55       |
| (1,1817) | 1:114:A:ARG:H   | 1:76:A:TRP:HE3  | 3                   | 1.65     | 0.58                | 1.48       |
| (1,1818) | 1:114:B:ARG:H   | 1:76:B:TRP:HE3  | 3                   | 1.65     | 0.58                | 1.48       |
| (1,2997) | 1:77:A:ASN:HD22 | 1:115:A:LYS:H   | 3                   | 1.26     | 1.03                | 0.72       |
| (1,369)  | 1:114:A:ARG:HB2 | 1:76:A:TRP:HE3  | 3                   | 1.26     | 0.76                | 1.37       |
| (1,370)  | 1:114:B:ARG:HB2 | 1:76:B:TRP:HE3  | 3                   | 1.26     | 0.76                | 1.37       |
| (1,2998) | 1:77:B:ASN:HD22 | 1:115:B:LYS:H   | 3                   | 1.25     | 1.03                | 0.71       |
| (1,2279) | 1:25:A:LYS:H    | 1:22:A:VAL:HG23 | 3                   | 1.23     | 0.2                 | 1.19       |
| (1,2279) | 1:25:A:LYS:H    | 1:22:A:VAL:HG21 | 3                   | 1.23     | 0.2                 | 1.19       |
| (1,2280) | 1:25:B:LYS:H    | 1:22:B:VAL:HG23 | 3                   | 1.23     | 0.2                 | 1.19       |
| (1,2280) | 1:25:B:LYS:H    | 1:22:B:VAL:HG21 | 3                   | 1.23     | 0.2                 | 1.19       |
| (3,5)    | 1:105:A:ASP:H   | 1:25:A:LYS:HG2  | 3                   | 1.21     | 0.42                | 1.28       |
| (3,6)    | 1:105:B:ASP:H   | 1:25:B:LYS:HG2  | 3                   | 1.21     | 0.42                | 1.28       |
| (1,1485) | 1:68:A:CYS:HB3  | 1:14:A:VAL:HG22 | 3                   | 1.21     | 1.28                | 0.47       |
| (1,1485) | 1:68:A:CYS:HB3  | 1:14:A:VAL:HG21 | 3                   | 1.21     | 1.28                | 0.47       |
| (1,1486) | 1:68:B:CYS:HB3  | 1:14:B:VAL:HG22 | 3                   | 1.21     | 1.28                | 0.47       |
| (1,1486) | 1:68:B:CYS:HB3  | 1:14:B:VAL:HG21 | 3                   | 1.21     | 1.28                | 0.47       |
| (1,1491) | 1:71:A:ILE:HD12 | 1:14:A:VAL:HG22 | 3                   | 1.2      | 1.01                | 0.68       |
| (1,1491) | 1:71:A:ILE:HD13 | 1:14:A:VAL:HG23 | 3                   | 1.2      | 1.01                | 0.68       |
| (1,1491) | 1:71:A:ILE:HD11 | 1:14:A:VAL:HG22 | 3                   | 1.2      | 1.01                | 0.68       |
| (1,1492) | 1:71:B:ILE:HD12 | 1:14:B:VAL:HG22 | 3                   | 1.2      | 1.01                | 0.68       |
| (1,1492) | 1:71:B:ILE:HD13 | 1:14:B:VAL:HG23 | 3                   | 1.2      | 1.01                | 0.68       |
| (1,1492) | 1:71:B:ILE:HD11 | 1:14:B:VAL:HG22 | 3                   | 1.2      | 1.01                | 0.68       |
| (1,1273) | 1:71:A:ILE:HD12 | 1:68:A:CYS:HB2  | 3                   | 1.07     | 0.39                | 1.21       |
| (1,1273) | 1:71:A:ILE:HD13 | 1:68:A:CYS:HB2  | 3                   | 1.07     | 0.39                | 1.21       |
| (1,1274) | 1:71:B:ILE:HD12 | 1:68:B:CYS:HB2  | 3                   | 1.07     | 0.4                 | 1.22       |
| (1,1274) | 1:71:B:ILE:HD13 | 1:68:B:CYS:HB2  | 3                   | 1.07     | 0.4                 | 1.22       |
| (1,308)  | 1:71:B:ILE:HG23 | 1:76:B:TRP:HB3  | 3                   | 1.03     | 1.08                | 0.37       |
| (1,308)  | 1:71:B:ILE:HG21 | 1:76:B:TRP:HB3  | 3                   | 1.03     | 1.08                | 0.37       |
| (1,308)  | 1:71:B:ILE:HG22 | 1:76:B:TRP:HB3  | 3                   | 1.03     | 1.08                | 0.37       |
| (1,307)  | 1:71:A:ILE:HG23 | 1:76:A:TRP:HB3  | 3                   | 1.03     | 1.08                | 0.37       |
| (1,307)  | 1:71:A:ILE:HG21 | 1:76:A:TRP:HB3  | 3                   | 1.03     | 1.08                | 0.37       |
| (1,307)  | 1:71:A:ILE:HG22 | 1:76:A:TRP:HB3  | 3                   | 1.03     | 1.08                | 0.37       |
| (1,667)  | 1:42:A:VAL:HG11 | 1:99:A:TRP:HZ2  | 3                   | 0.92     | 0.18                | 0.94       |
| (1,667)  | 1:42:A:VAL:HG12 | 1:99:A:TRP:HZ2  | 3                   | 0.92     | 0.18                | 0.94       |
| (1,667)  | 1:42:A:VAL:HG13 | 1:99:A:TRP:HZ2  | 3                   | 0.92     | 0.18                | 0.94       |
| (1,668)  | 1:42:B:VAL:HG11 | 1:99:B:TRP:HZ2  | 3                   | 0.92     | 0.18                | 0.94       |
| (1,668)  | 1:42:B:VAL:HG12 | 1:99:B:TRP:HZ2  | 3                   | 0.92     | 0.18                | 0.94       |
| (1,668)  | 1:42:B:VAL:HG13 | 1:99:B:TRP:HZ2  | 3                   | 0.92     | 0.18                | 0.94       |
| (1,2073) | 1:88:A:LYS:H    | 1:88:A:LYS:HB2  | 3                   | 0.85     | 0.04                | 0.86       |
| (1,2074) | 1:88:B:LYS:H    | 1:88:B:LYS:HB2  | 3                   | 0.85     | 0.04                | 0.86       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,926)  | 1:111:B:VAL:HG12 | 1:79:B:TYR:HE1  | 3                   | 0.85     | 0.54                | 0.7        |
| (1,926)  | 1:111:B:VAL:HG11 | 1:79:B:TYR:HE1  | 3                   | 0.85     | 0.54                | 0.7        |
| (1,925)  | 1:111:A:VAL:HG12 | 1:79:A:TYR:HE1  | 3                   | 0.85     | 0.53                | 0.7        |
| (1,925)  | 1:111:A:VAL:HG11 | 1:79:A:TYR:HE1  | 3                   | 0.85     | 0.53                | 0.7        |
| (1,2298) | 1:98:B:ALA:H     | 1:97:B:ALA:HB1  | 3                   | 0.81     | 0.19                | 0.94       |
| (1,2298) | 1:98:B:ALA:H     | 1:97:B:ALA:HB3  | 3                   | 0.81     | 0.19                | 0.94       |
| (1,2297) | 1:98:A:ALA:H     | 1:97:A:ALA:HB1  | 3                   | 0.81     | 0.18                | 0.93       |
| (1,2297) | 1:98:A:ALA:H     | 1:97:A:ALA:HB3  | 3                   | 0.81     | 0.18                | 0.93       |
| (1,2852) | 1:73:B:SER:H     | 1:71:B:ILE:HG21 | 3                   | 0.8      | 0.35                | 0.57       |
| (1,2852) | 1:73:B:SER:H     | 1:71:B:ILE:HG23 | 3                   | 0.8      | 0.35                | 0.57       |
| (1,2851) | 1:73:A:SER:H     | 1:71:A:ILE:HG21 | 3                   | 0.8      | 0.35                | 0.56       |
| (1,2851) | 1:73:A:SER:H     | 1:71:A:ILE:HG23 | 3                   | 0.8      | 0.35                | 0.56       |
| (1,2254) | 1:77:B:ASN:HD22  | 1:114:B:ARG:HA  | 3                   | 0.79     | 0.53                | 0.7        |
| (1,2253) | 1:77:A:ASN:HD22  | 1:114:A:ARG:HA  | 3                   | 0.79     | 0.52                | 0.69       |
| (1,1710) | 1:76:B:TRP:H     | 1:71:B:ILE:HG21 | 3                   | 0.72     | 0.46                | 0.52       |
| (1,1710) | 1:76:B:TRP:H     | 1:71:B:ILE:HG22 | 3                   | 0.72     | 0.46                | 0.52       |
| (1,1710) | 1:76:B:TRP:H     | 1:71:B:ILE:HG23 | 3                   | 0.72     | 0.46                | 0.52       |
| (1,1709) | 1:76:A:TRP:H     | 1:71:A:ILE:HG21 | 3                   | 0.71     | 0.45                | 0.52       |
| (1,1709) | 1:76:A:TRP:H     | 1:71:A:ILE:HG22 | 3                   | 0.71     | 0.45                | 0.52       |
| (1,1709) | 1:76:A:TRP:H     | 1:71:A:ILE:HG23 | 3                   | 0.71     | 0.45                | 0.52       |
| (1,1925) | 1:72:A:ASP:H     | 1:71:A:ILE:HD12 | 3                   | 0.61     | 0.34                | 0.66       |
| (1,1925) | 1:72:A:ASP:H     | 1:71:A:ILE:HD13 | 3                   | 0.61     | 0.34                | 0.66       |
| (1,1926) | 1:72:B:ASP:H     | 1:71:B:ILE:HD12 | 3                   | 0.6      | 0.35                | 0.66       |
| (1,1926) | 1:72:B:ASP:H     | 1:71:B:ILE:HD13 | 3                   | 0.6      | 0.35                | 0.66       |
| (1,2313) | 1:96:A:GLN:HE21  | 1:95:A:LYS:HA   | 3                   | 0.55     | 0.08                | 0.56       |
| (1,2314) | 1:96:B:GLN:HE21  | 1:95:B:LYS:HA   | 3                   | 0.55     | 0.07                | 0.56       |
| (1,437)  | 1:74:A:LYS:HG2   | 1:74:A:LYS:HE2  | 3                   | 0.53     | 0.02                | 0.53       |
| (1,438)  | 1:74:B:LYS:HG2   | 1:74:B:LYS:HE2  | 3                   | 0.53     | 0.02                | 0.53       |
| (1,2730) | 1:84:B:HIS:H     | 1:83:B:THR:HG23 | 3                   | 0.51     | 0.02                | 0.5        |
| (1,2730) | 1:84:B:HIS:H     | 1:83:B:THR:HG21 | 3                   | 0.51     | 0.02                | 0.5        |
| (1,2729) | 1:84:A:HIS:H     | 1:83:A:THR:HG23 | 3                   | 0.51     | 0.02                | 0.5        |
| (1,2729) | 1:84:A:HIS:H     | 1:83:A:THR:HG21 | 3                   | 0.51     | 0.02                | 0.5        |
| (1,54)   | 1:42:B:VAL:HG22  | 1:99:B:TRP:HZ2  | 3                   | 0.48     | 0.18                | 0.43       |
| (1,54)   | 1:42:B:VAL:HG23  | 1:99:B:TRP:HZ2  | 3                   | 0.48     | 0.18                | 0.43       |
| (1,53)   | 1:42:A:VAL:HG22  | 1:99:A:TRP:HZ2  | 3                   | 0.47     | 0.18                | 0.43       |
| (1,53)   | 1:42:A:VAL:HG23  | 1:99:A:TRP:HZ2  | 3                   | 0.47     | 0.18                | 0.43       |
| (1,1605) | 1:24:A:ASP:H     | 1:25:A:LYS:H    | 3                   | 0.42     | 0.2                 | 0.32       |
| (1,1606) | 1:24:B:ASP:H     | 1:25:B:LYS:H    | 3                   | 0.42     | 0.2                 | 0.32       |
| (1,1207) | 1:37:A:MET:HB2   | 1:26:A:THR:HG21 | 3                   | 0.35     | 0.18                | 0.28       |
| (1,1208) | 1:37:B:MET:HB2   | 1:26:B:THR:HG21 | 3                   | 0.35     | 0.18                | 0.28       |
| (1,1777) | 1:20:A:VAL:H     | 1:20:A:VAL:HG12 | 3                   | 0.35     | 0.13                | 0.3        |
| (1,1777) | 1:20:A:VAL:H     | 1:20:A:VAL:HG11 | 3                   | 0.35     | 0.13                | 0.3        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1778) | 1:20:B:VAL:H     | 1:20:B:VAL:HG12  | 3                   | 0.34     | 0.13                | 0.29       |
| (1,1778) | 1:20:B:VAL:H     | 1:20:B:VAL:HG11  | 3                   | 0.34     | 0.13                | 0.29       |
| (1,873)  | 1:39:A:LEU:HD12  | 1:91:A:THR:HA    | 3                   | 0.28     | 0.05                | 0.27       |
| (1,873)  | 1:39:A:LEU:HD13  | 1:91:A:THR:HA    | 3                   | 0.28     | 0.05                | 0.27       |
| (1,3040) | 1:35:B:GLU:H     | 1:34:B:LYS:HD3   | 3                   | 0.26     | 0.11                | 0.29       |
| (1,3039) | 1:35:A:GLU:H     | 1:34:A:LYS:HD3   | 3                   | 0.26     | 0.11                | 0.28       |
| (1,272)  | 1:14:B:VAL:HG12  | 1:15:B:CYS:HB2   | 3                   | 0.2      | 0.08                | 0.19       |
| (1,272)  | 1:14:B:VAL:HG11  | 1:15:B:CYS:HB2   | 3                   | 0.2      | 0.08                | 0.19       |
| (1,272)  | 1:14:B:VAL:HG13  | 1:15:B:CYS:HB2   | 3                   | 0.2      | 0.08                | 0.19       |
| (1,271)  | 1:14:A:VAL:HG12  | 1:15:A:CYS:HB2   | 3                   | 0.2      | 0.08                | 0.18       |
| (1,271)  | 1:14:A:VAL:HG11  | 1:15:A:CYS:HB2   | 3                   | 0.2      | 0.08                | 0.18       |
| (1,271)  | 1:14:A:VAL:HG13  | 1:15:A:CYS:HB2   | 3                   | 0.2      | 0.08                | 0.18       |
| (1,1555) | 1:49:A:PHE:HA    | 1:48:A:VAL:HB    | 3                   | 0.19     | 0.09                | 0.13       |
| (1,1556) | 1:49:B:PHE:HA    | 1:48:B:VAL:HB    | 3                   | 0.18     | 0.09                | 0.13       |
| (1,2579) | 1:107:A:ALA:H    | 1:82:A:THR:HG21  | 3                   | 0.18     | 0.05                | 0.19       |
| (1,2579) | 1:107:A:ALA:H    | 1:82:A:THR:HG23  | 3                   | 0.18     | 0.05                | 0.19       |
| (1,2580) | 1:107:B:ALA:H    | 1:82:B:THR:HG21  | 3                   | 0.18     | 0.05                | 0.19       |
| (1,2580) | 1:107:B:ALA:H    | 1:82:B:THR:HG23  | 3                   | 0.18     | 0.05                | 0.19       |
| (1,1266) | 1:70:B:GLY:HA2   | 1:71:B:ILE:HD11  | 3                   | 0.13     | 0.01                | 0.12       |
| (1,1266) | 1:70:B:GLY:HA2   | 1:71:B:ILE:HD12  | 3                   | 0.13     | 0.01                | 0.12       |
| (1,1265) | 1:70:A:GLY:HA2   | 1:71:A:ILE:HD11  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1265) | 1:70:A:GLY:HA2   | 1:71:A:ILE:HD12  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,3019) | 1:28:A:ALA:H     | 1:28:A:ALA:HB3   | 3                   | 0.13     | 0.01                | 0.12       |
| (1,3019) | 1:28:A:ALA:H     | 1:28:A:ALA:HB2   | 3                   | 0.13     | 0.01                | 0.12       |
| (1,227)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:H     | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,228)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:H     | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,3020) | 1:28:B:ALA:H     | 1:28:B:ALA:HB3   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,3020) | 1:28:B:ALA:H     | 1:28:B:ALA:HB2   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1472) | 1:112:B:LEU:HD21 | 1:112:B:LEU:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1472) | 1:112:B:LEU:HD21 | 1:112:B:LEU:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1471) | 1:112:A:LEU:HD21 | 1:112:A:LEU:HD13 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1471) | 1:112:A:LEU:HD21 | 1:112:A:LEU:HD11 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,750)  | 1:67:B:GLY:H     | 1:64:B:VAL:HG23  | 2                   | 2.81     | 0.41                | 2.81       |
| (1,750)  | 1:67:B:GLY:H     | 1:64:B:VAL:HG21  | 2                   | 2.81     | 0.41                | 2.81       |
| (1,749)  | 1:67:A:GLY:H     | 1:64:A:VAL:HG23  | 2                   | 2.8      | 0.4                 | 2.8        |
| (1,749)  | 1:67:A:GLY:H     | 1:64:A:VAL:HG21  | 2                   | 2.8      | 0.4                 | 2.8        |
| (1,2843) | 1:74:A:LYS:H     | 1:72:A:ASP:HB2   | 2                   | 1.08     | 0.57                | 1.08       |
| (1,2844) | 1:74:B:LYS:H     | 1:72:B:ASP:HB2   | 2                   | 1.08     | 0.57                | 1.08       |
| (1,1119) | 1:64:A:VAL:HG23  | 1:65:A:ASP:HB2   | 2                   | 1.04     | 0.02                | 1.04       |
| (1,1119) | 1:64:A:VAL:HG22  | 1:65:A:ASP:HB2   | 2                   | 1.04     | 0.02                | 1.04       |
| (1,1120) | 1:64:B:VAL:HG23  | 1:65:B:ASP:HB2   | 2                   | 1.04     | 0.02                | 1.04       |
| (1,1120) | 1:64:B:VAL:HG22  | 1:65:B:ASP:HB2   | 2                   | 1.04     | 0.02                | 1.04       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,688)  | 1:55:B:GLU:H     | 1:20:B:VAL:HG22 | 2                   | 0.84     | 0.66                | 0.84       |
| (1,688)  | 1:55:B:GLU:H     | 1:20:B:VAL:HG23 | 2                   | 0.84     | 0.66                | 0.84       |
| (1,687)  | 1:55:A:GLU:H     | 1:20:A:VAL:HG22 | 2                   | 0.84     | 0.66                | 0.84       |
| (1,687)  | 1:55:A:GLU:H     | 1:20:A:VAL:HG23 | 2                   | 0.84     | 0.66                | 0.84       |
| (1,1019) | 1:12:A:PHE:HB3   | 1:13:A:SER:HB2  | 2                   | 0.62     | 0.19                | 0.62       |
| (1,1020) | 1:12:B:PHE:HB3   | 1:13:B:SER:HB2  | 2                   | 0.61     | 0.19                | 0.61       |
| (1,597)  | 1:107:A:ALA:HB1  | 1:83:A:THR:HA   | 2                   | 0.6      | 0.4                 | 0.6        |
| (1,597)  | 1:107:A:ALA:HB2  | 1:83:A:THR:HA   | 2                   | 0.6      | 0.4                 | 0.6        |
| (1,598)  | 1:107:B:ALA:HB1  | 1:83:B:THR:HA   | 2                   | 0.59     | 0.4                 | 0.59       |
| (1,598)  | 1:107:B:ALA:HB2  | 1:83:B:THR:HA   | 2                   | 0.59     | 0.4                 | 0.59       |
| (1,2155) | 1:77:A:ASN:H     | 1:114:A:ARG:HA  | 2                   | 0.56     | 0.27                | 0.56       |
| (1,2156) | 1:77:B:ASN:H     | 1:114:B:ARG:HA  | 2                   | 0.56     | 0.26                | 0.56       |
| (1,1481) | 1:112:A:LEU:HD11 | 1:76:A:TRP:HB2  | 2                   | 0.55     | 0.19                | 0.55       |
| (1,1481) | 1:112:A:LEU:HD13 | 1:76:A:TRP:HB2  | 2                   | 0.55     | 0.19                | 0.55       |
| (1,1482) | 1:112:B:LEU:HD11 | 1:76:B:TRP:HB2  | 2                   | 0.54     | 0.18                | 0.54       |
| (1,1482) | 1:112:B:LEU:HD13 | 1:76:B:TRP:HB2  | 2                   | 0.54     | 0.18                | 0.54       |
| (1,2842) | 1:74:B:LYS:H     | 1:74:B:LYS:HD2  | 2                   | 0.49     | 0.04                | 0.49       |
| (1,2841) | 1:74:A:LYS:H     | 1:74:A:LYS:HD2  | 2                   | 0.48     | 0.04                | 0.48       |
| (1,2850) | 1:72:B:ASP:H     | 1:73:B:SER:H    | 2                   | 0.48     | 0.09                | 0.48       |
| (1,1027) | 1:18:A:VAL:HA    | 1:19:A:SER:HB2  | 2                   | 0.48     | 0.01                | 0.48       |
| (1,2849) | 1:72:A:ASP:H     | 1:73:A:SER:H    | 2                   | 0.47     | 0.08                | 0.47       |
| (1,1028) | 1:18:B:VAL:HA    | 1:19:B:SER:HB2  | 2                   | 0.47     | 0.01                | 0.47       |
| (1,193)  | 1:81:A:THR:HG21  | 1:79:A:TYR:HE1  | 2                   | 0.44     | 0.15                | 0.44       |
| (1,193)  | 1:81:A:THR:HG23  | 1:79:A:TYR:HE1  | 2                   | 0.44     | 0.15                | 0.44       |
| (1,659)  | 1:51:A:GLN:H     | 1:42:A:VAL:HG13 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,659)  | 1:51:A:GLN:H     | 1:42:A:VAL:HG11 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,660)  | 1:51:B:GLN:H     | 1:42:B:VAL:HG13 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,660)  | 1:51:B:GLN:H     | 1:42:B:VAL:HG11 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,194)  | 1:81:B:THR:HG21  | 1:79:B:TYR:HE1  | 2                   | 0.43     | 0.14                | 0.43       |
| (1,194)  | 1:81:B:THR:HG23  | 1:79:B:TYR:HE1  | 2                   | 0.43     | 0.14                | 0.43       |
| (1,183)  | 1:94:A:GLY:HA2   | 1:95:A:LYS:HB2  | 2                   | 0.43     | 0.02                | 0.43       |
| (1,184)  | 1:94:B:GLY:HA2   | 1:95:B:LYS:HB2  | 2                   | 0.43     | 0.02                | 0.43       |
| (1,1882) | 1:21:B:TRP:H     | 1:21:B:TRP:HZ2  | 2                   | 0.4      | 0.26                | 0.4        |
| (1,1881) | 1:21:A:TRP:H     | 1:21:A:TRP:HZ2  | 2                   | 0.4      | 0.28                | 0.4        |
| (1,1375) | 1:74:A:LYS:HD2   | 1:74:A:LYS:HB2  | 2                   | 0.37     | 0.01                | 0.37       |
| (1,1376) | 1:74:B:LYS:HD2   | 1:74:B:LYS:HB2  | 2                   | 0.37     | 0.01                | 0.37       |
| (1,293)  | 1:106:A:THR:HG23 | 1:85:A:THR:HB   | 2                   | 0.34     | 0.18                | 0.34       |
| (1,293)  | 1:106:A:THR:HG22 | 1:85:A:THR:HB   | 2                   | 0.34     | 0.18                | 0.34       |
| (1,294)  | 1:106:B:THR:HG23 | 1:85:B:THR:HB   | 2                   | 0.34     | 0.18                | 0.34       |
| (1,294)  | 1:106:B:THR:HG22 | 1:85:B:THR:HB   | 2                   | 0.34     | 0.18                | 0.34       |
| (1,2168) | 1:46:B:ASN:HD21  | 1:45:B:ASN:HA   | 2                   | 0.34     | 0.18                | 0.34       |
| (1,2167) | 1:46:A:ASN:HD21  | 1:45:A:ASN:HA   | 2                   | 0.33     | 0.16                | 0.33       |

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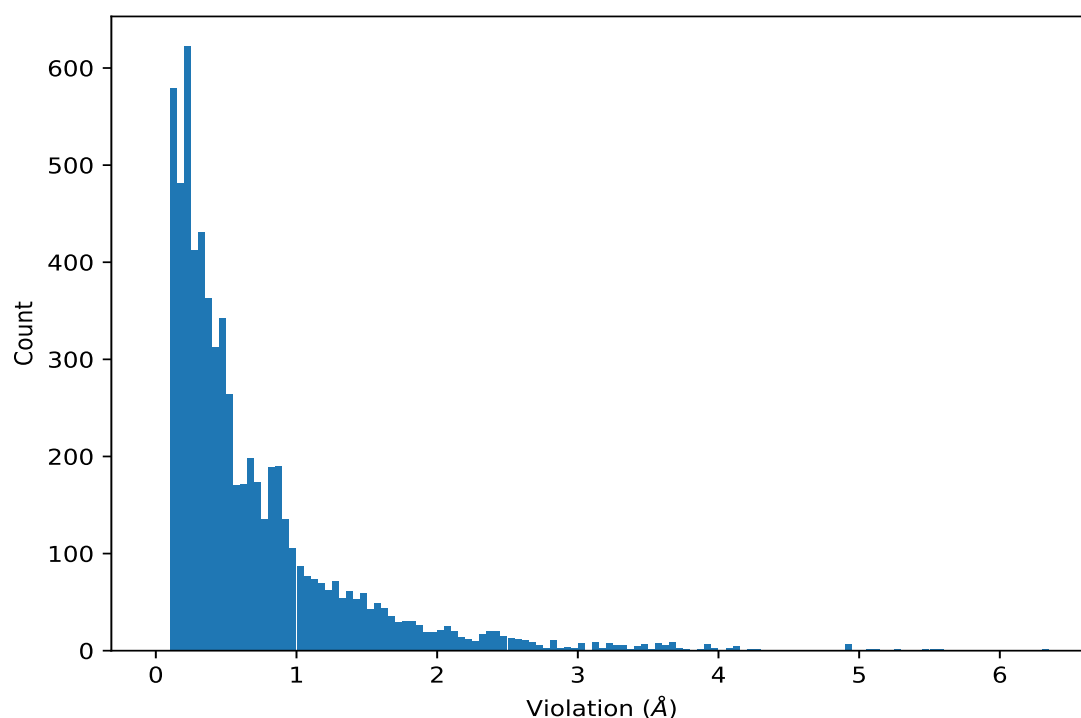
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,233)  | 1:33:A:GLY:HA2  | 1:29:A:THR:HB   | 2                   | 0.32     | 0.2                 | 0.32       |
| (1,234)  | 1:33:B:GLY:HA2  | 1:29:B:THR:HB   | 2                   | 0.32     | 0.2                 | 0.32       |
| (1,453)  | 1:95:A:LYS:HB2  | 1:95:A:LYS:HD2  | 2                   | 0.31     | 0.03                | 0.31       |
| (1,1161) | 1:95:A:LYS:H    | 1:95:A:LYS:HE3  | 2                   | 0.31     | 0.03                | 0.31       |
| (1,1162) | 1:95:B:LYS:H    | 1:95:B:LYS:HE3  | 2                   | 0.31     | 0.03                | 0.31       |
| (1,2329) | 1:75:A:HIS:H    | 1:74:A:LYS:H    | 2                   | 0.31     | 0.04                | 0.31       |
| (1,2330) | 1:75:B:HIS:H    | 1:74:B:LYS:H    | 2                   | 0.31     | 0.04                | 0.31       |
| (1,454)  | 1:95:B:LYS:HB2  | 1:95:B:LYS:HD2  | 2                   | 0.31     | 0.04                | 0.31       |
| (1,1718) | 1:76:B:TRP:H    | 1:74:B:LYS:HD2  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1087) | 1:115:A:LYS:HG2 | 1:114:A:ARG:HA  | 2                   | 0.27     | 0.13                | 0.27       |
| (1,1717) | 1:76:A:TRP:H    | 1:74:A:LYS:HD2  | 2                   | 0.27     | 0.13                | 0.27       |
| (1,1088) | 1:115:B:LYS:HG2 | 1:114:B:ARG:HA  | 2                   | 0.26     | 0.12                | 0.26       |
| (1,2431) | 1:92:A:MET:H    | 1:37:A:MET:HB2  | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2432) | 1:92:B:MET:H    | 1:37:B:MET:HB2  | 2                   | 0.16     | 0.06                | 0.16       |
| (1,2665) | 1:34:A:LYS:H    | 1:34:A:LYS:HD3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2666) | 1:34:B:LYS:H    | 1:34:B:LYS:HD3  | 2                   | 0.16     | 0.03                | 0.16       |
| (1,59)   | 1:42:A:VAL:HG21 | 1:49:A:PHE:HA   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,59)   | 1:42:A:VAL:HG23 | 1:49:A:PHE:HA   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,60)   | 1:42:B:VAL:HG21 | 1:49:B:PHE:HA   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,60)   | 1:42:B:VAL:HG23 | 1:49:B:PHE:HA   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,905)  | 1:9:A:ARG:H     | 1:9:A:ARG:HB2   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,906)  | 1:9:B:ARG:H     | 1:9:B:ARG:HB2   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1913) | 1:72:A:ASP:H    | 1:71:A:ILE:HA   | 2                   | 0.14     | 0.03                | 0.14       |
| (1,1914) | 1:72:B:ASP:H    | 1:71:B:ILE:HA   | 2                   | 0.14     | 0.03                | 0.14       |
| (1,339)  | 1:28:A:ALA:H    | 1:36:A:VAL:HG12 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,340)  | 1:28:B:ALA:H    | 1:36:B:VAL:HG12 | 2                   | 0.13     | 0.02                | 0.13       |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3100) | 1:9:B:ARG:HB3   | 1:117:A:VAL:HG21 | 10       | 6.35          |
| (1,3099) | 1:9:A:ARG:HB3   | 1:117:B:VAL:HG21 | 10       | 6.33          |
| (1,912)  | 1:9:B:ARG:HB2   | 1:6:B:ILE:HG13   | 9        | 5.57          |
| (1,911)  | 1:9:A:ARG:HB2   | 1:6:A:ILE:HG13   | 9        | 5.57          |
| (1,3102) | 1:9:B:ARG:HB3   | 1:115:A:LYS:HA   | 16       | 5.53          |
| (1,3101) | 1:9:A:ARG:HB3   | 1:115:B:LYS:HA   | 16       | 5.5           |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG11  | 12       | 5.48          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG11  | 12       | 5.47          |
| (1,550)  | 1:92:B:MET:HE1  | 1:97:B:ALA:HB1   | 15       | 5.25          |
| (1,549)  | 1:92:A:MET:HE1  | 1:97:A:ALA:HB1   | 15       | 5.25          |
| (1,2255) | 1:77:A:ASN:HD22 | 1:115:A:LYS:HG2  | 8        | 5.13          |
| (1,2256) | 1:77:B:ASN:HD22 | 1:115:B:LYS:HG2  | 8        | 5.1           |
| (1,3100) | 1:9:B:ARG:HB3   | 1:117:A:VAL:HG22 | 16       | 5.09          |
| (1,3099) | 1:9:A:ARG:HB3   | 1:117:B:VAL:HG22 | 16       | 5.05          |
| (1,3059) | 1:71:A:ILE:HD13 | 1:14:B:VAL:HB    | 20       | 4.95          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG12  | 15       | 4.93          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3053) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HG   | 6        | 4.92          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG12  | 15       | 4.92          |
| (1,3060) | 1:71:B:ILE:HD13 | 1:14:A:VAL:HB    | 20       | 4.91          |
| (1,1912) | 1:72:B:ASP:H    | 1:76:B:TRP:HB3   | 20       | 4.91          |
| (1,1911) | 1:72:A:ASP:H    | 1:76:A:TRP:HB3   | 20       | 4.91          |
| (1,3054) | 1:70:B:GLY:HA3  | 1:112:A:LEU:HG   | 6        | 4.9           |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG12  | 19       | 4.81          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG12  | 19       | 4.79          |
| (1,3073) | 1:114:A:ARG:H   | 1:12:B:PHE:HD2   | 20       | 4.43          |
| (1,3074) | 1:114:B:ARG:H   | 1:12:A:PHE:HD2   | 20       | 4.38          |
| (1,3061) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HD13 | 20       | 4.28          |
| (1,3062) | 1:70:B:GLY:HA3  | 1:112:A:LEU:HD13 | 20       | 4.26          |
| (1,3083) | 1:13:A:SER:H    | 1:111:B:VAL:HA   | 19       | 4.22          |
| (1,3084) | 1:13:B:SER:H    | 1:111:A:VAL:HA   | 19       | 4.2           |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG13  | 1        | 4.14          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG13  | 1        | 4.14          |
| (1,3067) | 1:70:A:GLY:HA3  | 1:71:B:ILE:HG22  | 6        | 4.12          |
| (1,3068) | 1:70:B:GLY:HA3  | 1:71:A:ILE:HG22  | 6        | 4.1           |
| (1,344)  | 1:48:B:VAL:HG11 | 1:41:B:GLU:HG2   | 19       | 4.1           |
| (1,343)  | 1:48:A:VAL:HG11 | 1:41:A:GLU:HG2   | 19       | 4.09          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG13  | 20       | 4.07          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG13  | 20       | 4.07          |
| (1,3084) | 1:13:B:SER:H    | 1:111:A:VAL:HA   | 15       | 3.97          |
| (1,550)  | 1:92:B:MET:HE2  | 1:97:B:ALA:HB3   | 9        | 3.96          |
| (1,549)  | 1:92:A:MET:HE2  | 1:97:A:ALA:HB3   | 9        | 3.95          |
| (1,3083) | 1:13:A:SER:H    | 1:111:B:VAL:HA   | 15       | 3.93          |
| (1,3083) | 1:13:A:SER:H    | 1:111:B:VAL:HA   | 8        | 3.92          |
| (1,3084) | 1:13:B:SER:H    | 1:111:A:VAL:HA   | 8        | 3.91          |
| (1,1490) | 1:110:B:CYS:HB3 | 1:14:B:VAL:HG22  | 16       | 3.91          |
| (1,1489) | 1:110:A:CYS:HB3 | 1:14:A:VAL:HG22  | 16       | 3.91          |
| (1,1204) | 1:37:B:MET:HE3  | 1:26:B:THR:HG21  | 8        | 3.91          |
| (1,1203) | 1:37:A:MET:HE3  | 1:26:A:THR:HG21  | 8        | 3.91          |
| (1,2552) | 1:76:B:TRP:HE1  | 1:75:B:HIS:HB2   | 20       | 3.85          |
| (1,2551) | 1:76:A:TRP:HE1  | 1:75:A:HIS:HB2   | 20       | 3.85          |
| (1,2552) | 1:76:B:TRP:HE1  | 1:75:B:HIS:HB2   | 17       | 3.78          |
| (1,2551) | 1:76:A:TRP:HE1  | 1:75:A:HIS:HB2   | 17       | 3.78          |
| (1,3083) | 1:13:A:SER:H    | 1:111:B:VAL:HA   | 11       | 3.74          |
| (1,3084) | 1:13:B:SER:H    | 1:111:A:VAL:HA   | 11       | 3.72          |
| (1,3102) | 1:9:B:ARG:HB3   | 1:115:A:LYS:HA   | 10       | 3.71          |
| (1,3060) | 1:71:B:ILE:HD12 | 1:14:A:VAL:HB    | 19       | 3.69          |
| (1,912)  | 1:9:B:ARG:HB2   | 1:6:B:ILE:HG13   | 12       | 3.68          |
| (1,911)  | 1:9:A:ARG:HB2   | 1:6:A:ILE:HG13   | 12       | 3.68          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3101) | 1:9:A:ARG:HB3   | 1:115:B:LYS:HA   | 10       | 3.67          |
| (1,3084) | 1:13:B:SER:H    | 1:111:A:VAL:HA   | 5        | 3.67          |
| (1,3083) | 1:13:A:SER:H    | 1:111:B:VAL:HA   | 5        | 3.66          |
| (1,2546) | 1:72:B:ASP:H    | 1:76:B:TRP:HE1   | 4        | 3.66          |
| (1,2545) | 1:72:A:ASP:H    | 1:76:A:TRP:HE1   | 4        | 3.66          |
| (1,3059) | 1:71:A:ILE:HD12 | 1:14:B:VAL:HB    | 19       | 3.65          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG13  | 9        | 3.63          |
| (1,3096) | 1:69:B:ARG:HA   | 1:112:A:LEU:HD21 | 19       | 3.62          |
| (1,1172) | 1:39:B:LEU:HD23 | 1:92:B:MET:HG2   | 19       | 3.62          |
| (1,1171) | 1:39:A:LEU:HD23 | 1:92:A:MET:HG2   | 19       | 3.62          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG13  | 9        | 3.61          |
| (1,3095) | 1:69:A:ARG:HA   | 1:112:B:LEU:HD21 | 19       | 3.6           |
| (1,3101) | 1:9:A:ARG:HB3   | 1:115:B:LYS:HA   | 17       | 3.58          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG12  | 2        | 3.57          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG12  | 2        | 3.57          |
| (1,3102) | 1:9:B:ARG:HB3   | 1:115:A:LYS:HA   | 17       | 3.56          |
| (1,1171) | 1:39:A:LEU:HD21 | 1:92:A:MET:HG2   | 1        | 3.56          |
| (1,1172) | 1:39:B:LEU:HD21 | 1:92:B:MET:HG2   | 1        | 3.55          |
| (1,344)  | 1:48:B:VAL:HG12 | 1:41:B:GLU:HG2   | 9        | 3.55          |
| (1,343)  | 1:48:A:VAL:HG12 | 1:41:A:GLU:HG2   | 9        | 3.55          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG12  | 16       | 3.51          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG12  | 16       | 3.5           |
| (1,1252) | 1:68:B:CYS:HB3  | 1:14:B:VAL:HB    | 11       | 3.48          |
| (1,1251) | 1:68:A:CYS:HB3  | 1:14:A:VAL:HB    | 11       | 3.48          |
| (1,912)  | 1:9:B:ARG:HB2   | 1:6:B:ILE:HG13   | 8        | 3.48          |
| (1,911)  | 1:9:A:ARG:HB2   | 1:6:A:ILE:HG13   | 8        | 3.47          |
| (1,226)  | 1:63:B:PRO:HB3  | 1:64:B:VAL:HG22  | 9        | 3.47          |
| (1,225)  | 1:63:A:PRO:HB3  | 1:64:A:VAL:HG22  | 9        | 3.47          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG11  | 13       | 3.45          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG11  | 13       | 3.44          |
| (1,3058) | 1:70:B:GLY:HA3  | 1:76:A:TRP:HE1   | 7        | 3.41          |
| (1,3057) | 1:70:A:GLY:HA3  | 1:76:B:TRP:HE1   | 7        | 3.41          |
| (1,344)  | 1:48:B:VAL:HG12 | 1:41:B:GLU:HG2   | 12       | 3.41          |
| (1,343)  | 1:48:A:VAL:HG12 | 1:41:A:GLU:HG2   | 12       | 3.41          |
| (1,2552) | 1:76:B:TRP:HE1  | 1:75:B:HIS:HB2   | 14       | 3.39          |
| (1,2551) | 1:76:A:TRP:HE1  | 1:75:A:HIS:HB2   | 14       | 3.39          |
| (1,908)  | 1:5:B:PRO:HA    | 1:9:B:ARG:HB2    | 14       | 3.33          |
| (1,907)  | 1:5:A:PRO:HA    | 1:9:A:ARG:HB2    | 14       | 3.33          |
| (1,886)  | 1:22:B:VAL:HB   | 1:53:B:PHE:HB3   | 8        | 3.33          |
| (1,885)  | 1:22:A:VAL:HB   | 1:53:A:PHE:HB3   | 8        | 3.33          |
| (1,3053) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HG   | 7        | 3.32          |
| (1,3054) | 1:70:B:GLY:HA3  | 1:112:A:LEU:HG   | 7        | 3.3           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG11  | 18       | 3.28          |
| (1,226)  | 1:63:B:PRO:HB3  | 1:64:B:VAL:HG23  | 14       | 3.27          |
| (1,225)  | 1:63:A:PRO:HB3  | 1:64:A:VAL:HG23  | 14       | 3.27          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG11  | 18       | 3.26          |
| (1,344)  | 1:48:B:VAL:HG11 | 1:41:B:GLU:HG2   | 5        | 3.26          |
| (1,343)  | 1:48:A:VAL:HG11 | 1:41:A:GLU:HG2   | 5        | 3.25          |
| (1,1204) | 1:37:B:MET:HE1  | 1:26:B:THR:HG21  | 20       | 3.22          |
| (1,750)  | 1:67:B:GLY:H    | 1:64:B:VAL:HG23  | 10       | 3.22          |
| (1,1203) | 1:37:A:MET:HE1  | 1:26:A:THR:HG21  | 20       | 3.21          |
| (1,907)  | 1:5:A:PRO:HA    | 1:9:A:ARG:HB2    | 19       | 3.21          |
| (1,749)  | 1:67:A:GLY:H    | 1:64:A:VAL:HG23  | 10       | 3.21          |
| (1,226)  | 1:63:B:PRO:HB3  | 1:64:B:VAL:HG23  | 2        | 3.21          |
| (1,225)  | 1:63:A:PRO:HB3  | 1:64:A:VAL:HG23  | 2        | 3.21          |
| (1,908)  | 1:5:B:PRO:HA    | 1:9:B:ARG:HB2    | 19       | 3.2           |
| (1,3099) | 1:9:A:ARG:HB3   | 1:117:B:VAL:HG23 | 2        | 3.19          |
| (3,8)    | 1:79:B:TYR:H    | 1:112:B:LEU:HD21 | 17       | 3.16          |
| (3,7)    | 1:79:A:TYR:H    | 1:112:A:LEU:HD21 | 17       | 3.16          |
| (1,3078) | 1:49:B:PHE:HE1  | 1:99:A:TRP:HE1   | 4        | 3.14          |
| (1,3060) | 1:71:B:ILE:HD12 | 1:14:A:VAL:HB    | 11       | 3.13          |
| (1,2560) | 1:76:B:TRP:HE1  | 1:112:B:LEU:HD12 | 14       | 3.13          |
| (1,2559) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HD12 | 14       | 3.13          |
| (1,3100) | 1:9:B:ARG:HB3   | 1:117:A:VAL:HG23 | 2        | 3.12          |
| (1,3077) | 1:49:A:PHE:HE1  | 1:99:B:TRP:HE1   | 4        | 3.12          |
| (1,3059) | 1:71:A:ILE:HD12 | 1:14:B:VAL:HB    | 11       | 3.12          |
| (1,1172) | 1:39:B:LEU:HD21 | 1:92:B:MET:HG2   | 8        | 3.11          |
| (1,1171) | 1:39:A:LEU:HD21 | 1:92:A:MET:HG2   | 8        | 3.11          |
| (1,3058) | 1:70:B:GLY:HA3  | 1:76:A:TRP:HE1   | 17       | 3.05          |
| (1,3096) | 1:69:B:ARG:HA   | 1:112:A:LEU:HD22 | 20       | 3.03          |
| (1,3095) | 1:69:A:ARG:HA   | 1:112:B:LEU:HD22 | 20       | 3.03          |
| (1,3057) | 1:70:A:GLY:HA3  | 1:76:B:TRP:HE1   | 17       | 3.03          |
| (1,1486) | 1:68:B:CYS:HB3  | 1:14:B:VAL:HG22  | 11       | 3.01          |
| (1,1485) | 1:68:A:CYS:HB3  | 1:14:A:VAL:HG22  | 11       | 3.01          |
| (1,1203) | 1:37:A:MET:HE2  | 1:26:A:THR:HG21  | 10       | 3.01          |
| (1,3099) | 1:9:A:ARG:HB3   | 1:117:B:VAL:HG21 | 13       | 3.0           |
| (1,1204) | 1:37:B:MET:HE2  | 1:26:B:THR:HG21  | 10       | 3.0           |
| (1,96)   | 1:22:B:VAL:HG11 | 1:53:B:PHE:HB3   | 8        | 2.98          |
| (1,95)   | 1:22:A:VAL:HG11 | 1:53:A:PHE:HB3   | 8        | 2.98          |
| (1,3067) | 1:70:A:GLY:HA3  | 1:71:B:ILE:HG21  | 19       | 2.95          |
| (1,3068) | 1:70:B:GLY:HA3  | 1:71:A:ILE:HG21  | 19       | 2.93          |
| (1,3058) | 1:70:B:GLY:HA2  | 1:76:A:TRP:HE1   | 6        | 2.92          |
| (1,3100) | 1:9:B:ARG:HB3   | 1:117:A:VAL:HG21 | 13       | 2.9           |
| (1,3057) | 1:70:A:GLY:HA2  | 1:76:B:TRP:HE1   | 6        | 2.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 5        | 2.86          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 7        | 2.85          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 5        | 2.85          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD21 | 14       | 2.84          |
| (1,908)  | 1:5:B:PRO:HA     | 1:9:B:ARG:HB2    | 5        | 2.84          |
| (1,907)  | 1:5:A:PRO:HA     | 1:9:A:ARG:HB2    | 5        | 2.84          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 20       | 2.83          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD22 | 17       | 2.83          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD21 | 14       | 2.83          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD22 | 17       | 2.83          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 7        | 2.83          |
| (1,2560) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD13 | 7        | 2.82          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 20       | 2.81          |
| (1,2559) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD13 | 7        | 2.81          |
| (1,3059) | 1:71:A:ILE:HD12  | 1:14:B:VAL:HB    | 7        | 2.79          |
| (1,3060) | 1:71:B:ILE:HD12  | 1:14:A:VAL:HB    | 7        | 2.78          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 5        | 2.75          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 5        | 2.74          |
| (1,3099) | 1:9:A:ARG:HB2    | 1:117:B:VAL:HG23 | 4        | 2.72          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21  | 8        | 2.72          |
| (1,2997) | 1:77:A:ASN:HD22  | 1:115:A:LYS:H    | 8        | 2.71          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21  | 8        | 2.71          |
| (1,3100) | 1:9:B:ARG:HB2    | 1:117:A:VAL:HG23 | 4        | 2.7           |
| (1,2998) | 1:77:B:ASN:HD22  | 1:115:B:LYS:H    | 8        | 2.69          |
| (1,3059) | 1:71:A:ILE:HD11  | 1:14:B:VAL:HB    | 16       | 2.68          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 7        | 2.68          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 7        | 2.68          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 8        | 2.68          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 8        | 2.68          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG11  | 17       | 2.68          |
| (1,3060) | 1:71:B:ILE:HD11  | 1:14:A:VAL:HB    | 16       | 2.67          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG11  | 17       | 2.66          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 6        | 2.64          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 6        | 2.64          |
| (1,3087) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HA    | 20       | 2.62          |
| (1,1492) | 1:71:B:ILE:HD12  | 1:14:B:VAL:HG22  | 16       | 2.62          |
| (1,1491) | 1:71:A:ILE:HD12  | 1:14:A:VAL:HG22  | 16       | 2.62          |
| (1,270)  | 1:14:B:VAL:HG13  | 1:110:B:CYS:HB3  | 17       | 2.62          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 5        | 2.61          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 5        | 2.61          |
| (1,356)  | 1:41:B:GLU:HG2   | 1:48:B:VAL:HA    | 19       | 2.61          |
| (1,269)  | 1:14:A:VAL:HG13  | 1:110:A:CYS:HB3  | 17       | 2.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,355)  | 1:41:A:GLU:HG2   | 1:48:A:VAL:HA    | 19       | 2.6           |
| (1,3089) | 1:112:A:LEU:HD22 | 1:14:B:VAL:HA    | 16       | 2.58          |
| (1,3088) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HA    | 20       | 2.58          |
| (1,3067) | 1:70:A:GLY:HA3   | 1:71:B:ILE:HG21  | 20       | 2.58          |
| (1,544)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD23  | 12       | 2.58          |
| (1,543)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD23  | 12       | 2.58          |
| (1,3090) | 1:112:B:LEU:HD22 | 1:14:A:VAL:HA    | 16       | 2.57          |
| (1,3068) | 1:70:B:GLY:HA3   | 1:71:A:ILE:HG21  | 20       | 2.57          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD13  | 14       | 2.56          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG12  | 7        | 2.56          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG12  | 7        | 2.55          |
| (1,308)  | 1:71:B:ILE:HG22  | 1:76:B:TRP:HB3   | 20       | 2.55          |
| (1,307)  | 1:71:A:ILE:HG22  | 1:76:A:TRP:HB3   | 20       | 2.55          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 1        | 2.54          |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD13  | 14       | 2.53          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 1        | 2.53          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 17       | 2.53          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 17       | 2.53          |
| (1,3087) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HA    | 16       | 2.52          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD21 | 19       | 2.51          |
| (1,251)  | 1:112:A:LEU:HD21 | 1:71:A:ILE:HA    | 20       | 2.51          |
| (1,3088) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HA    | 16       | 2.5           |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD21 | 19       | 2.5           |
| (1,252)  | 1:112:B:LEU:HD21 | 1:71:B:ILE:HA    | 20       | 2.5           |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG21  | 18       | 2.5           |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG21  | 18       | 2.5           |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD2   | 2        | 2.49          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 18       | 2.48          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 18       | 2.48          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 17       | 2.48          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 3        | 2.47          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD21 | 3        | 2.47          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 3        | 2.47          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 17       | 2.47          |
| (1,343)  | 1:48:A:VAL:HG11  | 1:41:A:GLU:HG2   | 1        | 2.47          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 3        | 2.46          |
| (1,344)  | 1:48:B:VAL:HG11  | 1:41:B:GLU:HG2   | 1        | 2.46          |
| (1,270)  | 1:14:B:VAL:HG11  | 1:110:B:CYS:HB3  | 16       | 2.46          |
| (1,269)  | 1:14:A:VAL:HG11  | 1:110:A:CYS:HB3  | 16       | 2.46          |
| (1,544)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD21  | 8        | 2.45          |
| (1,543)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD21  | 8        | 2.45          |
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD1   | 7        | 2.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 9        | 2.44          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 9        | 2.44          |
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG22 | 8        | 2.43          |
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD2   | 2        | 2.43          |
| (1,1818) | 1:114:B:ARG:H    | 1:76:B:TRP:HE3   | 7        | 2.43          |
| (1,1817) | 1:114:A:ARG:H    | 1:76:A:TRP:HE3   | 7        | 2.43          |
| (1,3080) | 1:11:B:GLU:HG2   | 1:111:A:VAL:HG22 | 8        | 2.42          |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD1   | 7        | 2.41          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG12  | 6        | 2.41          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG12  | 6        | 2.41          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 7        | 2.41          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 7        | 2.41          |
| (1,3059) | 1:71:A:ILE:HD11  | 1:14:B:VAL:HB    | 10       | 2.4           |
| (1,750)  | 1:67:B:GLY:H     | 1:64:B:VAL:HG21  | 11       | 2.4           |
| (1,749)  | 1:67:A:GLY:H     | 1:64:A:VAL:HG21  | 11       | 2.4           |
| (1,544)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD23  | 5        | 2.4           |
| (1,543)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD23  | 5        | 2.4           |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG21  | 4        | 2.4           |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG21  | 4        | 2.4           |
| (1,3099) | 1:9:A:ARG:HB2    | 1:117:B:VAL:HG21 | 11       | 2.38          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB2  | 8        | 2.38          |
| (1,424)  | 1:87:B:VAL:HG11  | 1:53:B:PHE:HD1   | 12       | 2.38          |
| (1,423)  | 1:87:A:VAL:HG11  | 1:53:A:PHE:HD1   | 12       | 2.38          |
| (1,550)  | 1:92:B:MET:HE1   | 1:97:B:ALA:HB2   | 18       | 2.37          |
| (1,549)  | 1:92:A:MET:HE1   | 1:97:A:ALA:HB2   | 18       | 2.37          |
| (1,3100) | 1:9:B:ARG:HB2    | 1:117:A:VAL:HG21 | 11       | 2.36          |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 10       | 2.36          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 18       | 2.36          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 18       | 2.36          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB2  | 8        | 2.36          |
| (1,3060) | 1:71:B:ILE:HD11  | 1:14:A:VAL:HB    | 10       | 2.36          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 5        | 2.36          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 5        | 2.36          |
| (1,426)  | 1:87:B:VAL:HG12  | 1:53:B:PHE:HE1   | 3        | 2.36          |
| (1,425)  | 1:87:A:VAL:HG12  | 1:53:A:PHE:HE1   | 3        | 2.36          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 4        | 2.35          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 4        | 2.35          |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 7        | 2.35          |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 7        | 2.35          |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG12 | 19       | 2.34          |
| (1,2552) | 1:76:B:TRP:HE1   | 1:75:B:HIS:HB2   | 7        | 2.34          |
| (1,2551) | 1:76:A:TRP:HE1   | 1:75:A:HIS:HB2   | 7        | 2.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG12  | 3        | 2.34          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG12  | 3        | 2.34          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 15       | 2.33          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 15       | 2.33          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG12 | 19       | 2.32          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 6        | 2.32          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 6        | 2.32          |
| (1,543)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD23  | 10       | 2.32          |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA    | 10       | 2.31          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 10       | 2.31          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 16       | 2.31          |
| (1,544)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD23  | 10       | 2.31          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 10       | 2.3           |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 16       | 2.3           |
| (1,2546) | 1:72:B:ASP:H     | 1:76:B:TRP:HE1   | 15       | 2.29          |
| (1,2545) | 1:72:A:ASP:H     | 1:76:A:TRP:HE1   | 15       | 2.29          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 6        | 2.29          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 6        | 2.29          |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 5        | 2.29          |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 5        | 2.29          |
| (1,3076) | 1:42:B:VAL:HG23  | 1:99:A:TRP:HE1   | 10       | 2.26          |
| (1,3075) | 1:42:A:VAL:HG23  | 1:99:B:TRP:HE1   | 10       | 2.25          |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG21  | 18       | 2.25          |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG21  | 18       | 2.25          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD23 | 6        | 2.24          |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB3   | 19       | 2.24          |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB3   | 19       | 2.24          |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD11  | 14       | 2.22          |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD11  | 14       | 2.22          |
| (1,3076) | 1:42:B:VAL:HG22  | 1:99:A:TRP:HE1   | 9        | 2.22          |
| (1,3075) | 1:42:A:VAL:HG22  | 1:99:B:TRP:HE1   | 9        | 2.22          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG11  | 5        | 2.22          |
| (1,4)    | 1:111:B:VAL:HG23 | 1:112:B:LEU:HD23 | 2        | 2.22          |
| (1,3)    | 1:111:A:VAL:HG23 | 1:112:A:LEU:HD23 | 2        | 2.22          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD23 | 6        | 2.21          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG11  | 5        | 2.21          |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 15       | 2.19          |
| (1,543)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD23  | 19       | 2.19          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 14       | 2.18          |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 15       | 2.18          |
| (1,544)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD23  | 19       | 2.18          |
| (1,3058) | 1:70:B:GLY:HA3   | 1:76:A:TRP:HE1   | 20       | 2.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3057) | 1:70:A:GLY:HA3  | 1:76:B:TRP:HE1   | 20       | 2.17          |
| (1,2544) | 1:76:B:TRP:HE1  | 1:112:B:LEU:HD23 | 13       | 2.17          |
| (1,2543) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HD23 | 13       | 2.16          |
| (1,3096) | 1:69:B:ARG:HA   | 1:112:A:LEU:HD21 | 14       | 2.15          |
| (1,960)  | 1:59:B:ARG:HD2  | 1:18:B:VAL:HB    | 9        | 2.15          |
| (1,959)  | 1:59:A:ARG:HD2  | 1:18:A:VAL:HB    | 9        | 2.15          |
| (1,922)  | 1:116:B:ALA:HB3 | 1:115:B:LYS:HA   | 15       | 2.15          |
| (1,921)  | 1:116:A:ALA:HB3 | 1:115:A:LYS:HA   | 15       | 2.15          |
| (1,3064) | 1:12:B:PHE:H    | 1:111:A:VAL:HG11 | 20       | 2.14          |
| (1,3102) | 1:9:B:ARG:HB2   | 1:115:A:LYS:HA   | 18       | 2.13          |
| (1,96)   | 1:22:B:VAL:HG12 | 1:53:B:PHE:HB3   | 17       | 2.13          |
| (1,61)   | 1:63:A:PRO:HD2  | 1:64:A:VAL:HG13  | 15       | 2.13          |
| (1,370)  | 1:114:B:ARG:HB2 | 1:76:B:TRP:HE3   | 14       | 2.12          |
| (1,369)  | 1:114:A:ARG:HB2 | 1:76:A:TRP:HE3   | 14       | 2.12          |
| (1,356)  | 1:41:B:GLU:HG2  | 1:48:B:VAL:HA    | 5        | 2.12          |
| (1,355)  | 1:41:A:GLU:HG2  | 1:48:A:VAL:HA    | 5        | 2.12          |
| (1,95)   | 1:22:A:VAL:HG12 | 1:53:A:PHE:HB3   | 17       | 2.12          |
| (1,62)   | 1:63:B:PRO:HD2  | 1:64:B:VAL:HG13  | 15       | 2.12          |
| (1,2370) | 1:29:B:THR:H    | 1:103:B:ARG:HG2  | 11       | 2.11          |
| (1,2369) | 1:29:A:THR:H    | 1:103:A:ARG:HG2  | 11       | 2.11          |
| (1,62)   | 1:63:B:PRO:HD2  | 1:64:B:VAL:HG13  | 7        | 2.11          |
| (1,61)   | 1:63:A:PRO:HD2  | 1:64:A:VAL:HG13  | 7        | 2.11          |
| (1,3080) | 1:11:B:GLU:HG2  | 1:111:A:VAL:HG21 | 5        | 2.1           |
| (1,3079) | 1:11:A:GLU:HG2  | 1:111:B:VAL:HG21 | 5        | 2.1           |
| (1,1995) | 1:67:A:GLY:H    | 1:64:A:VAL:HB    | 11       | 2.1           |
| (1,550)  | 1:92:B:MET:HE3  | 1:97:B:ALA:HB1   | 16       | 2.1           |
| (1,549)  | 1:92:A:MET:HE3  | 1:97:A:ALA:HB1   | 16       | 2.1           |
| (1,226)  | 1:63:B:PRO:HB3  | 1:64:B:VAL:HG22  | 11       | 2.1           |
| (1,3084) | 1:13:B:SER:H    | 1:111:A:VAL:HA   | 20       | 2.09          |
| (1,3083) | 1:13:A:SER:H    | 1:111:B:VAL:HA   | 20       | 2.09          |
| (1,3063) | 1:12:A:PHE:H    | 1:111:B:VAL:HG11 | 20       | 2.09          |
| (1,1996) | 1:67:B:GLY:H    | 1:64:B:VAL:HB    | 11       | 2.09          |
| (1,544)  | 1:92:B:MET:HE2  | 1:39:B:LEU:HD21  | 1        | 2.09          |
| (1,225)  | 1:63:A:PRO:HB3  | 1:64:A:VAL:HG22  | 11       | 2.09          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG12  | 14       | 2.08          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG12  | 14       | 2.08          |
| (1,543)  | 1:92:A:MET:HE2  | 1:39:A:LEU:HD21  | 1        | 2.08          |
| (1,3101) | 1:9:A:ARG:HB2   | 1:115:B:LYS:HA   | 18       | 2.07          |
| (1,922)  | 1:116:B:ALA:HB2 | 1:115:B:LYS:HA   | 20       | 2.07          |
| (1,921)  | 1:116:A:ALA:HB2 | 1:115:A:LYS:HA   | 20       | 2.07          |
| (1,886)  | 1:22:B:VAL:HB   | 1:53:B:PHE:HB3   | 20       | 2.07          |
| (1,885)  | 1:22:A:VAL:HB   | 1:53:A:PHE:HB3   | 20       | 2.07          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,544)  | 1:92:B:MET:HE1  | 1:39:B:LEU:HD21  | 11       | 2.07          |
| (1,543)  | 1:92:A:MET:HE1  | 1:39:A:LEU:HD21  | 11       | 2.07          |
| (1,1952) | 1:105:B:ASP:H   | 1:55:B:GLU:HB2   | 13       | 2.06          |
| (1,1951) | 1:105:A:ASP:H   | 1:55:A:GLU:HB2   | 13       | 2.06          |
| (1,2150) | 1:77:B:ASN:H    | 1:112:B:LEU:HD23 | 20       | 2.05          |
| (1,2149) | 1:77:A:ASN:H    | 1:112:A:LEU:HD23 | 20       | 2.05          |
| (1,1951) | 1:105:A:ASP:H   | 1:55:A:GLU:HB2   | 4        | 2.05          |
| (1,886)  | 1:22:B:VAL:HB   | 1:53:B:PHE:HB3   | 2        | 2.05          |
| (1,885)  | 1:22:A:VAL:HB   | 1:53:A:PHE:HB3   | 2        | 2.05          |
| (1,96)   | 1:22:B:VAL:HG13 | 1:53:B:PHE:HB3   | 9        | 2.05          |
| (1,95)   | 1:22:A:VAL:HG13 | 1:53:A:PHE:HB3   | 9        | 2.05          |
| (1,3061) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HD12 | 6        | 2.04          |
| (1,1952) | 1:105:B:ASP:H   | 1:55:B:GLU:HB2   | 4        | 2.04          |
| (1,1389) | 1:57:A:LYS:HE2  | 1:18:A:VAL:HG12  | 3        | 2.04          |
| (1,426)  | 1:87:B:VAL:HG11 | 1:53:B:PHE:HE1   | 12       | 2.04          |
| (1,270)  | 1:14:B:VAL:HG13 | 1:110:B:CYS:HB3  | 11       | 2.04          |
| (1,269)  | 1:14:A:VAL:HG13 | 1:110:A:CYS:HB3  | 11       | 2.04          |
| (1,1390) | 1:57:B:LYS:HE2  | 1:18:B:VAL:HG12  | 3        | 2.03          |
| (1,426)  | 1:87:B:VAL:HG11 | 1:53:B:PHE:HE1   | 20       | 2.03          |
| (1,425)  | 1:87:A:VAL:HG11 | 1:53:A:PHE:HE1   | 12       | 2.03          |
| (1,425)  | 1:87:A:VAL:HG11 | 1:53:A:PHE:HE1   | 20       | 2.03          |
| (1,424)  | 1:87:B:VAL:HG12 | 1:53:B:PHE:HD1   | 3        | 2.03          |
| (1,423)  | 1:87:A:VAL:HG12 | 1:53:A:PHE:HD1   | 3        | 2.03          |
| (1,3062) | 1:70:B:GLY:HA3  | 1:112:A:LEU:HD12 | 6        | 2.02          |
| (1,1215) | 1:22:A:VAL:HG13 | 1:20:A:VAL:HB    | 9        | 2.02          |
| (1,885)  | 1:22:A:VAL:HB   | 1:53:A:PHE:HB3   | 10       | 2.02          |
| (1,1216) | 1:22:B:VAL:HG13 | 1:20:B:VAL:HB    | 9        | 2.01          |
| (1,886)  | 1:22:B:VAL:HB   | 1:53:B:PHE:HB3   | 10       | 2.01          |
| (1,550)  | 1:92:B:MET:HE1  | 1:97:B:ALA:HB2   | 7        | 2.01          |
| (1,549)  | 1:92:A:MET:HE1  | 1:97:A:ALA:HB2   | 7        | 2.01          |
| (1,960)  | 1:59:B:ARG:HD2  | 1:18:B:VAL:HB    | 20       | 2.0           |
| (1,959)  | 1:59:A:ARG:HD2  | 1:18:A:VAL:HB    | 20       | 2.0           |
| (1,3101) | 1:9:A:ARG:HB3   | 1:115:B:LYS:HA   | 13       | 1.99          |
| (1,1844) | 1:96:B:GLN:HE22 | 1:95:B:LYS:HA    | 5        | 1.99          |
| (1,1843) | 1:96:A:GLN:HE22 | 1:95:A:LYS:HA    | 5        | 1.99          |
| (1,3054) | 1:70:B:GLY:HA3  | 1:112:A:LEU:HG   | 13       | 1.98          |
| (1,2544) | 1:76:B:TRP:HE1  | 1:112:B:LEU:HD21 | 10       | 1.98          |
| (1,2543) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HD21 | 10       | 1.98          |
| (1,960)  | 1:59:B:ARG:HD2  | 1:18:B:VAL:HB    | 4        | 1.98          |
| (1,343)  | 1:48:A:VAL:HG11 | 1:41:A:GLU:HG2   | 7        | 1.98          |
| (1,1886) | 1:21:B:TRP:H    | 1:54:B:PHE:HD1   | 16       | 1.97          |
| (1,1003) | 1:53:A:PHE:HB3  | 1:22:A:VAL:HG22  | 5        | 1.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 4        | 1.97          |
| (1,344)  | 1:48:B:VAL:HG11  | 1:41:B:GLU:HG2   | 7        | 1.97          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 14       | 1.96          |
| (1,1885) | 1:21:A:TRP:H     | 1:54:A:PHE:HD1   | 16       | 1.96          |
| (1,1494) | 1:68:B:CYS:HB2   | 1:14:B:VAL:HG22  | 11       | 1.96          |
| (1,1493) | 1:68:A:CYS:HB2   | 1:14:A:VAL:HG22  | 11       | 1.96          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG22  | 5        | 1.96          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 13       | 1.95          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 18       | 1.95          |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG13 | 11       | 1.94          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 14       | 1.94          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 18       | 1.94          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 18       | 1.94          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 18       | 1.94          |
| (1,544)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD23  | 13       | 1.92          |
| (1,137)  | 1:39:A:LEU:HG    | 1:92:A:MET:HG2   | 1        | 1.92          |
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD2   | 8        | 1.91          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG13 | 11       | 1.91          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 17       | 1.91          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 17       | 1.91          |
| (1,543)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD23  | 13       | 1.91          |
| (1,250)  | 1:112:B:LEU:HD22 | 1:76:B:TRP:HD1   | 17       | 1.91          |
| (1,249)  | 1:112:A:LEU:HD22 | 1:76:A:TRP:HD1   | 17       | 1.91          |
| (1,138)  | 1:39:B:LEU:HG    | 1:92:B:MET:HG2   | 1        | 1.91          |
| (1,3102) | 1:9:B:ARG:HB3    | 1:115:A:LYS:HA   | 13       | 1.9           |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 20       | 1.9           |
| (1,550)  | 1:92:B:MET:HE1   | 1:97:B:ALA:HB3   | 17       | 1.9           |
| (1,549)  | 1:92:A:MET:HE1   | 1:97:A:ALA:HB3   | 17       | 1.9           |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 20       | 1.89          |
| (1,1170) | 1:39:B:LEU:HD11  | 1:92:B:MET:HG2   | 1        | 1.89          |
| (1,1169) | 1:39:A:LEU:HD11  | 1:92:A:MET:HG2   | 1        | 1.89          |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD2   | 8        | 1.88          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 12       | 1.88          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 12       | 1.88          |
| (1,1314) | 1:70:B:GLY:H     | 1:64:B:VAL:HG12  | 12       | 1.88          |
| (1,1313) | 1:70:A:GLY:H     | 1:64:A:VAL:HG12  | 12       | 1.88          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 3        | 1.87          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 3        | 1.87          |
| (1,1996) | 1:67:B:GLY:H     | 1:64:B:VAL:HB    | 10       | 1.87          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG22  | 1        | 1.87          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG22  | 1        | 1.87          |
| (1,2560) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD13 | 17       | 1.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2559) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD13 | 17       | 1.86          |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG13  | 15       | 1.86          |
| (1,2501) | 1:69:A:ARG:H     | 1:64:A:VAL:HG13  | 15       | 1.86          |
| (1,1995) | 1:67:A:GLY:H     | 1:64:A:VAL:HB    | 10       | 1.86          |
| (1,544)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD23  | 4        | 1.86          |
| (1,543)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD23  | 4        | 1.86          |
| (1,1172) | 1:39:B:LEU:HD23  | 1:92:B:MET:HG2   | 12       | 1.85          |
| (1,1171) | 1:39:A:LEU:HD23  | 1:92:A:MET:HG2   | 12       | 1.85          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 15       | 1.85          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG23  | 12       | 1.85          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG23  | 12       | 1.85          |
| (1,179)  | 1:109:A:VAL:HG21 | 1:81:A:THR:HA    | 12       | 1.85          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 1        | 1.84          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 8        | 1.84          |
| (1,1449) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HE1   | 8        | 1.84          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 15       | 1.84          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 16       | 1.84          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 16       | 1.84          |
| (1,180)  | 1:109:B:VAL:HG21 | 1:81:B:THR:HA    | 12       | 1.84          |
| (1,180)  | 1:109:B:VAL:HG22 | 1:81:B:THR:HA    | 19       | 1.84          |
| (1,179)  | 1:109:A:VAL:HG22 | 1:81:A:THR:HA    | 19       | 1.84          |
| (1,4)    | 1:111:B:VAL:HG23 | 1:112:B:LEU:HD21 | 17       | 1.84          |
| (1,3)    | 1:111:A:VAL:HG23 | 1:112:A:LEU:HD21 | 17       | 1.84          |
| (1,3060) | 1:71:B:ILE:HD13  | 1:14:A:VAL:HB    | 9        | 1.83          |
| (1,3059) | 1:71:A:ILE:HD13  | 1:14:B:VAL:HB    | 9        | 1.83          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 8        | 1.83          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 8        | 1.83          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 4        | 1.83          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 4        | 1.83          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 1        | 1.82          |
| (1,1170) | 1:39:B:LEU:HD13  | 1:92:B:MET:HG2   | 19       | 1.82          |
| (1,1169) | 1:39:A:LEU:HD13  | 1:92:A:MET:HG2   | 19       | 1.82          |
| (1,3099) | 1:9:A:ARG:HB2    | 1:117:B:VAL:HG22 | 6        | 1.81          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG13  | 1        | 1.81          |
| (1,343)  | 1:48:A:VAL:HG12  | 1:41:A:GLU:HG2   | 17       | 1.81          |
| (1,3099) | 1:9:A:ARG:HB2    | 1:117:B:VAL:HG23 | 19       | 1.8           |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG11 | 1        | 1.8           |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG13  | 1        | 1.8           |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 8        | 1.8           |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 8        | 1.8           |
| (1,96)   | 1:22:B:VAL:HG12  | 1:53:B:PHE:HB3   | 20       | 1.8           |
| (1,95)   | 1:22:A:VAL:HG12  | 1:53:A:PHE:HB3   | 20       | 1.8           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3100) | 1:9:B:ARG:HB3    | 1:117:A:VAL:HG22 | 14       | 1.79          |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG11 | 1        | 1.79          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 5        | 1.79          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 5        | 1.79          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 5        | 1.79          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 13       | 1.79          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 13       | 1.79          |
| (1,344)  | 1:48:B:VAL:HG12  | 1:41:B:GLU:HG2   | 17       | 1.79          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 5        | 1.78          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 18       | 1.78          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 18       | 1.78          |
| (1,179)  | 1:109:A:VAL:HG22 | 1:81:A:THR:HA    | 16       | 1.78          |
| (1,3099) | 1:9:A:ARG:HB3    | 1:117:B:VAL:HG22 | 14       | 1.77          |
| (1,3085) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HG21  | 10       | 1.77          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG11 | 8        | 1.77          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG11 | 16       | 1.77          |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG11 | 16       | 1.77          |
| (1,922)  | 1:116:B:ALA:HB2  | 1:115:B:LYS:HA   | 7        | 1.77          |
| (1,549)  | 1:92:A:MET:HE3   | 1:97:A:ALA:HB3   | 13       | 1.77          |
| (1,180)  | 1:109:B:VAL:HG22 | 1:81:B:THR:HA    | 16       | 1.77          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 12       | 1.76          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 13       | 1.76          |
| (1,953)  | 1:18:A:VAL:HG23  | 1:59:A:ARG:HD2   | 9        | 1.76          |
| (1,921)  | 1:116:A:ALA:HB2  | 1:115:A:LYS:HA   | 7        | 1.76          |
| (1,550)  | 1:92:B:MET:HE3   | 1:97:B:ALA:HB3   | 13       | 1.76          |
| (1,3100) | 1:9:B:ARG:HB2    | 1:117:A:VAL:HG22 | 6        | 1.75          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 13       | 1.75          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG11  | 8        | 1.75          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG11  | 8        | 1.75          |
| (1,954)  | 1:18:B:VAL:HG23  | 1:59:B:ARG:HD2   | 9        | 1.75          |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG11 | 8        | 1.74          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 12       | 1.74          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG23  | 17       | 1.74          |
| (1,908)  | 1:5:B:PRO:HA     | 1:9:B:ARG:HB2    | 3        | 1.74          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG11  | 11       | 1.73          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG11  | 11       | 1.73          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG23  | 17       | 1.73          |
| (1,907)  | 1:5:A:PRO:HA     | 1:9:A:ARG:HB2    | 3        | 1.73          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG23  | 13       | 1.73          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG23  | 13       | 1.73          |
| (1,3086) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HG21  | 10       | 1.72          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 3        | 1.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 7        | 1.72          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 7        | 1.72          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG11  | 17       | 1.72          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG11  | 17       | 1.72          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 3        | 1.71          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 12       | 1.71          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 12       | 1.71          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 5        | 1.71          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 5        | 1.71          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG12  | 13       | 1.71          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG12  | 13       | 1.71          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21  | 7        | 1.71          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21  | 7        | 1.71          |
| (1,96)   | 1:22:B:VAL:HG13  | 1:53:B:PHE:HB3   | 2        | 1.71          |
| (1,95)   | 1:22:A:VAL:HG13  | 1:53:A:PHE:HB3   | 2        | 1.71          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 1        | 1.7           |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 1        | 1.7           |
| (3,6)    | 1:105:B:ASP:H    | 1:25:B:LYS:HG2   | 14       | 1.69          |
| (3,5)    | 1:105:A:ASP:H    | 1:25:A:LYS:HG2   | 14       | 1.69          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 17       | 1.69          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 17       | 1.69          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 4        | 1.69          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 4        | 1.69          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG13  | 11       | 1.69          |
| (1,1204) | 1:37:B:MET:HE3   | 1:26:B:THR:HG23  | 13       | 1.69          |
| (1,1170) | 1:39:B:LEU:HD13  | 1:92:B:MET:HG2   | 8        | 1.69          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 20       | 1.69          |
| (1,3100) | 1:9:B:ARG:HB2    | 1:117:A:VAL:HG23 | 19       | 1.68          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG13  | 11       | 1.68          |
| (1,1203) | 1:37:A:MET:HE3   | 1:26:A:THR:HG23  | 13       | 1.68          |
| (1,1169) | 1:39:A:LEU:HD13  | 1:92:A:MET:HG2   | 8        | 1.68          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 20       | 1.68          |
| (1,179)  | 1:109:A:VAL:HG21 | 1:81:A:THR:HA    | 4        | 1.68          |
| (1,3102) | 1:9:B:ARG:HB3    | 1:115:A:LYS:HA   | 7        | 1.67          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 1        | 1.67          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 1        | 1.67          |
| (1,356)  | 1:41:B:GLU:HG2   | 1:48:B:VAL:HA    | 9        | 1.67          |
| (1,355)  | 1:41:A:GLU:HG2   | 1:48:A:VAL:HA    | 9        | 1.67          |
| (1,180)  | 1:109:B:VAL:HG21 | 1:81:B:THR:HA    | 4        | 1.67          |
| (1,180)  | 1:109:B:VAL:HG21 | 1:81:B:THR:HA    | 15       | 1.67          |
| (1,179)  | 1:109:A:VAL:HG21 | 1:81:A:THR:HA    | 15       | 1.67          |
| (3,2)    | 1:52:B:TYR:HB2   | 1:22:B:VAL:HB    | 15       | 1.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,1)    | 1:52:A:TYR:HB2   | 1:22:A:VAL:HB    | 15       | 1.66          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 15       | 1.66          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 15       | 1.66          |
| (1,544)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD22  | 16       | 1.66          |
| (1,543)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD22  | 16       | 1.66          |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 6        | 1.66          |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 6        | 1.66          |
| (1,3101) | 1:9:A:ARG:HB3    | 1:115:B:LYS:HA   | 7        | 1.65          |
| (1,2844) | 1:74:B:LYS:H     | 1:72:B:ASP:HB2   | 20       | 1.65          |
| (1,2843) | 1:74:A:LYS:H     | 1:72:A:ASP:HB2   | 20       | 1.65          |
| (1,252)  | 1:112:B:LEU:HD22 | 1:71:B:ILE:HA    | 17       | 1.65          |
| (1,3058) | 1:70:B:GLY:HA3   | 1:76:A:TRP:HE1   | 2        | 1.64          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 2        | 1.64          |
| (1,2608) | 1:107:B:ALA:H    | 1:56:B:THR:HG21  | 15       | 1.64          |
| (1,2607) | 1:107:A:ALA:H    | 1:56:A:THR:HG21  | 15       | 1.64          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 9        | 1.64          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 9        | 1.64          |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 19       | 1.64          |
| (1,251)  | 1:112:A:LEU:HD22 | 1:71:A:ILE:HA    | 17       | 1.64          |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 19       | 1.64          |
| (3,8)    | 1:79:B:TYR:H     | 1:112:B:LEU:HD22 | 18       | 1.63          |
| (3,7)    | 1:79:A:TYR:H     | 1:112:A:LEU:HD22 | 18       | 1.63          |
| (1,3102) | 1:9:B:ARG:HB3    | 1:115:A:LYS:HA   | 1        | 1.63          |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA    | 19       | 1.63          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG22  | 9        | 1.63          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG22  | 9        | 1.63          |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG13  | 12       | 1.63          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG13  | 12       | 1.63          |
| (1,780)  | 1:106:B:THR:HB   | 1:85:B:THR:HG22  | 16       | 1.62          |
| (1,779)  | 1:106:A:THR:HB   | 1:85:A:THR:HG22  | 16       | 1.62          |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 5        | 1.62          |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 5        | 1.62          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB2  | 9        | 1.61          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG22  | 18       | 1.61          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 8        | 1.61          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 8        | 1.61          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 15       | 1.61          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 15       | 1.61          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG12  | 19       | 1.61          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 2        | 1.61          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB2  | 9        | 1.6           |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG22  | 18       | 1.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 16       | 1.6           |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 16       | 1.6           |
| (1,1885) | 1:21:A:TRP:H     | 1:54:A:PHE:HD1   | 2        | 1.6           |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG12  | 19       | 1.6           |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 2        | 1.6           |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 19       | 1.6           |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 19       | 1.6           |
| (1,550)  | 1:92:B:MET:HE1   | 1:97:B:ALA:HB3   | 3        | 1.6           |
| (1,549)  | 1:92:A:MET:HE1   | 1:97:A:ALA:HB3   | 3        | 1.6           |
| (1,336)  | 1:36:B:VAL:HG12  | 1:30:B:ASP:HB2   | 5        | 1.6           |
| (1,335)  | 1:36:A:VAL:HG12  | 1:30:A:ASP:HB2   | 5        | 1.6           |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG21  | 15       | 1.6           |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG21  | 15       | 1.6           |
| (1,3101) | 1:9:A:ARG:HB3    | 1:115:B:LYS:HA   | 1        | 1.59          |
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD2   | 1        | 1.59          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 1        | 1.59          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 1        | 1.59          |
| (1,1886) | 1:21:B:TRP:H     | 1:54:B:PHE:HD1   | 2        | 1.59          |
| (1,1886) | 1:21:B:TRP:H     | 1:54:B:PHE:HD1   | 5        | 1.59          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD23 | 14       | 1.58          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD23 | 14       | 1.58          |
| (1,1885) | 1:21:A:TRP:H     | 1:54:A:PHE:HD1   | 5        | 1.58          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 17       | 1.58          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG22  | 5        | 1.58          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG22  | 6        | 1.58          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG22  | 5        | 1.58          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG22  | 6        | 1.58          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 13       | 1.58          |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 19       | 1.57          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 5        | 1.57          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 12       | 1.57          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 12       | 1.57          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG23  | 17       | 1.57          |
| (1,926)  | 1:111:B:VAL:HG12 | 1:79:B:TYR:HE1   | 16       | 1.57          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA   | 17       | 1.57          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 1        | 1.57          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 1        | 1.57          |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 13       | 1.57          |
| (1,3087) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HA    | 7        | 1.56          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 2        | 1.56          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 5        | 1.56          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 2        | 1.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 5        | 1.56          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 5        | 1.56          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 16       | 1.56          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG23  | 17       | 1.56          |
| (1,925)  | 1:111:A:VAL:HG12 | 1:79:A:TYR:HE1   | 16       | 1.56          |
| (1,662)  | 1:42:B:VAL:HG12  | 1:90:B:LEU:HG    | 19       | 1.56          |
| (1,661)  | 1:42:A:VAL:HG12  | 1:90:A:LEU:HG    | 19       | 1.56          |
| (1,542)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD12  | 12       | 1.56          |
| (1,541)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD12  | 12       | 1.56          |
| (1,356)  | 1:41:B:GLU:HG2   | 1:48:B:VAL:HA    | 12       | 1.56          |
| (1,138)  | 1:39:B:LEU:HG    | 1:92:B:MET:HG2   | 8        | 1.56          |
| (1,3088) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HA    | 7        | 1.55          |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD2   | 1        | 1.55          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 16       | 1.55          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 14       | 1.55          |
| (1,355)  | 1:41:A:GLU:HG2   | 1:48:A:VAL:HA    | 12       | 1.55          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 8        | 1.55          |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 8        | 1.55          |
| (1,138)  | 1:39:B:LEU:HG    | 1:92:B:MET:HG2   | 19       | 1.55          |
| (1,137)  | 1:39:A:LEU:HG    | 1:92:A:MET:HG2   | 8        | 1.55          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 11       | 1.54          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 11       | 1.54          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 16       | 1.54          |
| (1,1544) | 1:55:B:GLU:HG3   | 1:20:B:VAL:HG23  | 9        | 1.54          |
| (1,1543) | 1:55:A:GLU:HG3   | 1:20:A:VAL:HG23  | 9        | 1.54          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 11       | 1.54          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 11       | 1.54          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 14       | 1.54          |
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG22  | 4        | 1.54          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG22  | 4        | 1.54          |
| (1,137)  | 1:39:A:LEU:HG    | 1:92:A:MET:HG2   | 19       | 1.54          |
| (3,2)    | 1:52:B:TYR:HB2   | 1:51:B:GLN:HG3   | 14       | 1.53          |
| (3,1)    | 1:52:A:TYR:HB2   | 1:51:A:GLN:HG3   | 14       | 1.53          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG22  | 6        | 1.53          |
| (1,2255) | 1:77:A:ASN:HD22  | 1:115:A:LYS:HG2  | 18       | 1.53          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 16       | 1.53          |
| (1,954)  | 1:18:B:VAL:HG21  | 1:59:B:ARG:HD2   | 5        | 1.53          |
| (1,953)  | 1:18:A:VAL:HG21  | 1:59:A:ARG:HD2   | 5        | 1.53          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 1        | 1.53          |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 1        | 1.53          |
| (1,3059) | 1:71:A:ILE:HD11  | 1:14:B:VAL:HB    | 15       | 1.52          |
| (1,2552) | 1:76:B:TRP:HE1   | 1:75:B:HIS:HB2   | 9        | 1.52          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2551) | 1:76:A:TRP:HE1  | 1:75:A:HIS:HB2   | 9        | 1.52          |
| (1,2548) | 1:76:B:TRP:HE1  | 1:71:B:ILE:HG22  | 6        | 1.52          |
| (1,2544) | 1:76:B:TRP:HE1  | 1:112:B:LEU:HD22 | 4        | 1.52          |
| (1,2543) | 1:76:A:TRP:HE1  | 1:112:A:LEU:HD22 | 4        | 1.52          |
| (1,2256) | 1:77:B:ASN:HD22 | 1:115:B:LYS:HG2  | 18       | 1.52          |
| (1,2150) | 1:77:B:ASN:H    | 1:112:B:LEU:HD22 | 11       | 1.52          |
| (1,2149) | 1:77:A:ASN:H    | 1:112:A:LEU:HD22 | 11       | 1.52          |
| (1,1436) | 1:38:B:VAL:HG21 | 1:28:B:ALA:HB1   | 13       | 1.52          |
| (1,1435) | 1:38:A:VAL:HG21 | 1:28:A:ALA:HB1   | 13       | 1.52          |
| (1,1399) | 1:59:A:ARG:HG2  | 1:18:A:VAL:HG12  | 10       | 1.52          |
| (1,550)  | 1:92:B:MET:HE3  | 1:97:B:ALA:HB3   | 11       | 1.52          |
| (1,549)  | 1:92:A:MET:HE3  | 1:97:A:ALA:HB3   | 11       | 1.52          |
| (1,3083) | 1:13:A:SER:H    | 1:111:B:VAL:HA   | 3        | 1.51          |
| (1,2150) | 1:77:B:ASN:H    | 1:112:B:LEU:HD22 | 15       | 1.51          |
| (1,2149) | 1:77:A:ASN:H    | 1:112:A:LEU:HD22 | 15       | 1.51          |
| (1,1400) | 1:59:B:ARG:HG2  | 1:18:B:VAL:HG12  | 10       | 1.51          |
| (1,3084) | 1:13:B:SER:H    | 1:111:A:VAL:HA   | 3        | 1.5           |
| (1,2812) | 1:81:B:THR:H    | 1:79:B:TYR:HB2   | 18       | 1.5           |
| (1,2811) | 1:81:A:THR:H    | 1:79:A:TYR:HB2   | 18       | 1.5           |
| (1,688)  | 1:55:B:GLU:H    | 1:20:B:VAL:HG22  | 9        | 1.5           |
| (1,47)   | 1:42:A:VAL:HG23 | 1:44:A:ILE:HB    | 10       | 1.5           |
| (1,3060) | 1:71:B:ILE:HD11 | 1:14:A:VAL:HB    | 15       | 1.49          |
| (1,2502) | 1:69:B:ARG:H    | 1:64:B:VAL:HG12  | 11       | 1.49          |
| (1,2280) | 1:25:B:LYS:H    | 1:22:B:VAL:HG21  | 7        | 1.49          |
| (1,2279) | 1:25:A:LYS:H    | 1:22:A:VAL:HG21  | 7        | 1.49          |
| (1,908)  | 1:5:B:PRO:HA    | 1:9:B:ARG:HB2    | 16       | 1.49          |
| (1,687)  | 1:55:A:GLU:H    | 1:20:A:VAL:HG22  | 9        | 1.49          |
| (1,544)  | 1:92:B:MET:HE3  | 1:39:B:LEU:HD21  | 3        | 1.49          |
| (1,426)  | 1:87:B:VAL:HG11 | 1:53:B:PHE:HE1   | 13       | 1.49          |
| (1,425)  | 1:87:A:VAL:HG11 | 1:53:A:PHE:HE1   | 13       | 1.49          |
| (1,270)  | 1:14:B:VAL:HG13 | 1:110:B:CYS:HB3  | 7        | 1.49          |
| (1,269)  | 1:14:A:VAL:HG13 | 1:110:A:CYS:HB3  | 7        | 1.49          |
| (1,48)   | 1:42:B:VAL:HG23 | 1:44:B:ILE:HB    | 10       | 1.49          |
| (1,2812) | 1:81:B:THR:H    | 1:79:B:TYR:HB2   | 14       | 1.48          |
| (1,2811) | 1:81:A:THR:H    | 1:79:A:TYR:HB2   | 14       | 1.48          |
| (1,2501) | 1:69:A:ARG:H    | 1:64:A:VAL:HG12  | 11       | 1.48          |
| (1,2254) | 1:77:B:ASN:HD22 | 1:114:B:ARG:HA   | 18       | 1.48          |
| (1,1818) | 1:114:B:ARG:H   | 1:76:B:TRP:HE3   | 14       | 1.48          |
| (1,1817) | 1:114:A:ARG:H   | 1:76:A:TRP:HE3   | 14       | 1.48          |
| (1,1400) | 1:59:B:ARG:HG2  | 1:18:B:VAL:HG13  | 7        | 1.48          |
| (1,1400) | 1:59:B:ARG:HG2  | 1:18:B:VAL:HG13  | 14       | 1.48          |
| (1,1399) | 1:59:A:ARG:HG2  | 1:18:A:VAL:HG13  | 14       | 1.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1172) | 1:39:B:LEU:HD23  | 1:92:B:MET:HG2   | 5        | 1.48          |
| (1,907)  | 1:5:A:PRO:HA     | 1:9:A:ARG:HB2    | 16       | 1.48          |
| (1,543)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD21  | 3        | 1.48          |
| (1,96)   | 1:22:B:VAL:HG13  | 1:53:B:PHE:HB3   | 6        | 1.48          |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 13       | 1.48          |
| (1,95)   | 1:22:A:VAL:HG13  | 1:53:A:PHE:HB3   | 6        | 1.48          |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 13       | 1.48          |
| (1,4)    | 1:111:B:VAL:HG23 | 1:112:B:LEU:HD23 | 20       | 1.48          |
| (1,3)    | 1:111:A:VAL:HG23 | 1:112:A:LEU:HD23 | 20       | 1.48          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD22 | 1        | 1.47          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD22 | 1        | 1.47          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 19       | 1.47          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 10       | 1.47          |
| (1,2253) | 1:77:A:ASN:HD22  | 1:114:A:ARG:HA   | 18       | 1.47          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 6        | 1.47          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG13  | 7        | 1.47          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG13  | 8        | 1.47          |
| (1,1314) | 1:70:B:GLY:H     | 1:64:B:VAL:HG11  | 6        | 1.47          |
| (1,1313) | 1:70:A:GLY:H     | 1:64:A:VAL:HG11  | 6        | 1.47          |
| (1,1274) | 1:71:B:ILE:HD12  | 1:68:B:CYS:HB2   | 16       | 1.47          |
| (1,1273) | 1:71:A:ILE:HD12  | 1:68:A:CYS:HB2   | 16       | 1.47          |
| (1,1171) | 1:39:A:LEU:HD23  | 1:92:A:MET:HG2   | 5        | 1.47          |
| (1,922)  | 1:116:B:ALA:HB1  | 1:115:B:LYS:HA   | 13       | 1.47          |
| (1,921)  | 1:116:A:ALA:HB1  | 1:115:A:LYS:HA   | 13       | 1.47          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 12       | 1.47          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 12       | 1.47          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 16       | 1.46          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 13       | 1.46          |
| (1,2608) | 1:107:B:ALA:H    | 1:56:B:THR:HG22  | 19       | 1.46          |
| (1,2607) | 1:107:A:ALA:H    | 1:56:A:THR:HG22  | 19       | 1.46          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 10       | 1.46          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 19       | 1.46          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 6        | 1.46          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG13  | 8        | 1.46          |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 10       | 1.45          |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 10       | 1.45          |
| (1,662)  | 1:42:B:VAL:HG12  | 1:90:B:LEU:HG    | 17       | 1.45          |
| (1,661)  | 1:42:A:VAL:HG12  | 1:90:A:LEU:HG    | 17       | 1.45          |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG22  | 13       | 1.44          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 6        | 1.44          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 1        | 1.44          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 1        | 1.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB1   | 6        | 1.44          |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB1   | 6        | 1.44          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 16       | 1.43          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 9        | 1.43          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 8        | 1.43          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG22  | 13       | 1.43          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD21 | 9        | 1.43          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 6        | 1.43          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD21 | 9        | 1.43          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 19       | 1.43          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG21  | 10       | 1.43          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG21  | 10       | 1.43          |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 10       | 1.43          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 13       | 1.42          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 9        | 1.42          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 8        | 1.42          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 9        | 1.42          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 5        | 1.42          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 5        | 1.42          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 12       | 1.42          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 12       | 1.42          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG11  | 13       | 1.42          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 19       | 1.42          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG23  | 17       | 1.42          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG23  | 17       | 1.42          |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 10       | 1.42          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 9        | 1.41          |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 19       | 1.41          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 12       | 1.41          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 12       | 1.41          |
| (1,550)  | 1:92:B:MET:HE3   | 1:97:B:ALA:HB3   | 1        | 1.41          |
| (1,549)  | 1:92:A:MET:HE3   | 1:97:A:ALA:HB3   | 1        | 1.41          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG11  | 13       | 1.41          |
| (1,315)  | 1:71:A:ILE:HG23  | 1:76:A:TRP:HB2   | 20       | 1.41          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG21  | 19       | 1.41          |
| (1,96)   | 1:22:B:VAL:HG13  | 1:53:B:PHE:HB3   | 11       | 1.41          |
| (1,95)   | 1:22:A:VAL:HG13  | 1:53:A:PHE:HB3   | 11       | 1.41          |
| (1,3099) | 1:9:A:ARG:HB3    | 1:117:B:VAL:HG21 | 8        | 1.4           |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD22 | 2        | 1.4           |
| (1,3075) | 1:42:A:VAL:HG22  | 1:99:B:TRP:HE1   | 18       | 1.4           |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG11 | 2        | 1.4           |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 19       | 1.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 7        | 1.4           |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 7        | 1.4           |
| (1,316)  | 1:71:B:ILE:HG23  | 1:76:B:TRP:HB2   | 20       | 1.4           |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG21  | 19       | 1.4           |
| (1,96)   | 1:22:B:VAL:HG12  | 1:53:B:PHE:HB3   | 15       | 1.4           |
| (1,4)    | 1:111:B:VAL:HG22 | 1:112:B:LEU:HD22 | 16       | 1.4           |
| (1,3)    | 1:111:A:VAL:HG22 | 1:112:A:LEU:HD22 | 16       | 1.4           |
| (1,3076) | 1:42:B:VAL:HG22  | 1:99:A:TRP:HE1   | 18       | 1.39          |
| (1,3060) | 1:71:B:ILE:HD11  | 1:14:A:VAL:HB    | 8        | 1.39          |
| (1,3059) | 1:71:A:ILE:HD11  | 1:14:B:VAL:HB    | 8        | 1.39          |
| (1,1886) | 1:21:B:TRP:H     | 1:54:B:PHE:HD1   | 17       | 1.39          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG21  | 16       | 1.39          |
| (1,96)   | 1:22:B:VAL:HG12  | 1:53:B:PHE:HB3   | 18       | 1.39          |
| (1,95)   | 1:22:A:VAL:HG12  | 1:53:A:PHE:HB3   | 15       | 1.39          |
| (1,95)   | 1:22:A:VAL:HG12  | 1:53:A:PHE:HB3   | 18       | 1.39          |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG13 | 2        | 1.38          |
| (1,3052) | 1:21:B:TRP:HE1   | 1:31:A:ILE:HD12  | 10       | 1.38          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG21 | 11       | 1.38          |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 18       | 1.38          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 18       | 1.38          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 18       | 1.38          |
| (1,1885) | 1:21:A:TRP:H     | 1:54:A:PHE:HD1   | 17       | 1.38          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 8        | 1.38          |
| (1,424)  | 1:87:B:VAL:HG11  | 1:53:B:PHE:HD1   | 20       | 1.38          |
| (1,423)  | 1:87:A:VAL:HG11  | 1:53:A:PHE:HD1   | 20       | 1.38          |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 13       | 1.38          |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 13       | 1.38          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG21  | 16       | 1.38          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 17       | 1.38          |
| (1,3100) | 1:9:B:ARG:HB3    | 1:117:A:VAL:HG21 | 8        | 1.37          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 12       | 1.37          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG21 | 11       | 1.37          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 8        | 1.37          |
| (1,370)  | 1:114:B:ARG:HB2  | 1:76:B:TRP:HE3   | 17       | 1.37          |
| (1,369)  | 1:114:A:ARG:HB2  | 1:76:A:TRP:HE3   | 17       | 1.37          |
| (1,180)  | 1:109:B:VAL:HG21 | 1:81:B:THR:HA    | 9        | 1.37          |
| (1,179)  | 1:109:A:VAL:HG21 | 1:81:A:THR:HA    | 9        | 1.37          |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 17       | 1.37          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD22 | 2        | 1.36          |
| (1,3051) | 1:21:A:TRP:HE1   | 1:31:B:ILE:HD12  | 10       | 1.36          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 12       | 1.36          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD22 | 9        | 1.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 4        | 1.36          |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 4        | 1.36          |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 7        | 1.36          |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 18       | 1.36          |
| (1,2096) | 1:68:B:CYS:H     | 1:71:B:ILE:HB    | 10       | 1.36          |
| (1,2095) | 1:68:A:CYS:H     | 1:71:A:ILE:HB    | 10       | 1.36          |
| (1,1962) | 1:43:B:ASN:HD21  | 1:48:B:VAL:HG11  | 12       | 1.36          |
| (1,1961) | 1:43:A:ASN:HD21  | 1:48:A:VAL:HG11  | 12       | 1.36          |
| (1,356)  | 1:41:B:GLU:HG2   | 1:48:B:VAL:HA    | 1        | 1.36          |
| (1,355)  | 1:41:A:GLU:HG2   | 1:48:A:VAL:HA    | 1        | 1.36          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD22 | 9        | 1.35          |
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 7        | 1.35          |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 6        | 1.35          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 6        | 1.35          |
| (1,1910) | 1:72:B:ASP:H     | 1:71:B:ILE:HG21  | 5        | 1.35          |
| (1,1909) | 1:72:A:ASP:H     | 1:71:A:ILE:HG21  | 5        | 1.35          |
| (1,1710) | 1:76:B:TRP:H     | 1:71:B:ILE:HG23  | 7        | 1.35          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 9        | 1.35          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 9        | 1.35          |
| (1,886)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HB3   | 3        | 1.35          |
| (1,550)  | 1:92:B:MET:HE3   | 1:97:B:ALA:HB3   | 2        | 1.35          |
| (1,549)  | 1:92:A:MET:HE3   | 1:97:A:ALA:HB3   | 2        | 1.35          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 3        | 1.35          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 6        | 1.35          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 3        | 1.35          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 6        | 1.35          |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA    | 9        | 1.34          |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 9        | 1.34          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 4        | 1.34          |
| (1,1709) | 1:76:A:TRP:H     | 1:71:A:ILE:HG23  | 7        | 1.34          |
| (1,1476) | 1:112:B:LEU:HD12 | 1:71:B:ILE:HA    | 14       | 1.34          |
| (1,1475) | 1:112:A:LEU:HD12 | 1:71:A:ILE:HA    | 14       | 1.34          |
| (1,885)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HB3   | 3        | 1.34          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG23  | 20       | 1.34          |
| (1,3101) | 1:9:A:ARG:HB3    | 1:115:B:LYS:HA   | 2        | 1.33          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 1        | 1.33          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 1        | 1.33          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 4        | 1.33          |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG21  | 17       | 1.33          |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG21  | 17       | 1.33          |
| (1,756)  | 1:103:B:ARG:HD2  | 1:86:B:PHE:HE1   | 5        | 1.33          |
| (1,755)  | 1:103:A:ARG:HD2  | 1:86:A:PHE:HE1   | 5        | 1.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,270)  | 1:14:B:VAL:HG13  | 1:110:B:CYS:HB3  | 10       | 1.33          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG23  | 20       | 1.33          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 2        | 1.32          |
| (1,2551) | 1:76:A:TRP:HE1   | 1:75:A:HIS:HB2   | 19       | 1.32          |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 2        | 1.32          |
| (1,1130) | 1:77:B:ASN:HB2   | 1:113:B:SER:HB2  | 8        | 1.32          |
| (1,1129) | 1:77:A:ASN:HB2   | 1:113:A:SER:HB2  | 8        | 1.32          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 13       | 1.32          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 13       | 1.32          |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB2   | 4        | 1.32          |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB2   | 4        | 1.32          |
| (1,269)  | 1:14:A:VAL:HG13  | 1:110:A:CYS:HB3  | 10       | 1.32          |
| (1,2552) | 1:76:B:TRP:HE1   | 1:75:B:HIS:HB2   | 19       | 1.31          |
| (1,2369) | 1:29:A:THR:H     | 1:103:A:ARG:HG2  | 15       | 1.31          |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 13       | 1.31          |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 2        | 1.31          |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 13       | 1.31          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB1   | 13       | 1.31          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB1   | 13       | 1.31          |
| (1,1331) | 1:64:A:VAL:HG22  | 1:65:A:ASP:HB3   | 20       | 1.31          |
| (3,2)    | 1:52:B:TYR:HB2   | 1:51:B:GLN:HG3   | 11       | 1.3           |
| (3,1)    | 1:52:A:TYR:HB2   | 1:51:A:GLN:HG3   | 11       | 1.3           |
| (1,3086) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HG23  | 7        | 1.3           |
| (1,3085) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HG23  | 7        | 1.3           |
| (1,2852) | 1:73:B:SER:H     | 1:71:B:ILE:HG23  | 7        | 1.3           |
| (1,2851) | 1:73:A:SER:H     | 1:71:A:ILE:HG23  | 7        | 1.3           |
| (1,2370) | 1:29:B:THR:H     | 1:103:B:ARG:HG2  | 15       | 1.3           |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 19       | 1.3           |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 19       | 1.3           |
| (1,1332) | 1:64:B:VAL:HG22  | 1:65:B:ASP:HB3   | 20       | 1.3           |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 15       | 1.3           |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 5        | 1.3           |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 15       | 1.3           |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG13 | 20       | 1.3           |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG13 | 20       | 1.3           |
| (1,180)  | 1:109:B:VAL:HG22 | 1:81:B:THR:HA    | 7        | 1.3           |
| (1,179)  | 1:109:A:VAL:HG22 | 1:81:A:THR:HA    | 7        | 1.3           |
| (1,95)   | 1:22:A:VAL:HG12  | 1:53:A:PHE:HB3   | 14       | 1.3           |
| (1,1172) | 1:39:B:LEU:HD22  | 1:92:B:MET:HG2   | 16       | 1.29          |
| (1,1171) | 1:39:A:LEU:HD22  | 1:92:A:MET:HG2   | 16       | 1.29          |
| (1,1130) | 1:77:B:ASN:HB2   | 1:113:B:SER:HB2  | 9        | 1.29          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 5        | 1.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,544)  | 1:92:B:MET:HE2  | 1:39:B:LEU:HD21  | 20       | 1.29          |
| (1,96)   | 1:22:B:VAL:HG12 | 1:53:B:PHE:HB3   | 14       | 1.29          |
| (3,6)    | 1:105:B:ASP:H   | 1:25:B:LYS:HG2   | 11       | 1.28          |
| (3,5)    | 1:105:A:ASP:H   | 1:25:A:LYS:HG2   | 11       | 1.28          |
| (1,1129) | 1:77:A:ASN:HB2  | 1:113:A:SER:HB2  | 9        | 1.28          |
| (1,1064) | 1:57:B:LYS:HD2  | 1:57:B:LYS:HB2   | 11       | 1.28          |
| (1,1063) | 1:57:A:LYS:HD2  | 1:57:A:LYS:HB2   | 11       | 1.28          |
| (1,922)  | 1:116:B:ALA:HB3 | 1:115:B:LYS:HA   | 12       | 1.28          |
| (1,921)  | 1:116:A:ALA:HB3 | 1:115:A:LYS:HA   | 12       | 1.28          |
| (1,543)  | 1:92:A:MET:HE2  | 1:39:A:LEU:HD21  | 20       | 1.28          |
| (1,542)  | 1:92:B:MET:HE3  | 1:39:B:LEU:HD12  | 8        | 1.28          |
| (1,541)  | 1:92:A:MET:HE3  | 1:39:A:LEU:HD12  | 8        | 1.28          |
| (1,3079) | 1:11:A:GLU:HG2  | 1:111:B:VAL:HG22 | 15       | 1.27          |
| (1,3070) | 1:11:B:GLU:H    | 1:113:A:SER:HB3  | 18       | 1.27          |
| (1,2150) | 1:77:B:ASN:H    | 1:112:B:LEU:HD22 | 10       | 1.27          |
| (1,2149) | 1:77:A:ASN:H    | 1:112:A:LEU:HD22 | 10       | 1.27          |
| (1,1420) | 1:6:B:ILE:HG12  | 1:6:B:ILE:HG22   | 20       | 1.27          |
| (1,1400) | 1:59:B:ARG:HG2  | 1:18:B:VAL:HG11  | 20       | 1.27          |
| (1,1399) | 1:59:A:ARG:HG2  | 1:18:A:VAL:HG11  | 20       | 1.27          |
| (1,1172) | 1:39:B:LEU:HD23 | 1:92:B:MET:HG2   | 10       | 1.27          |
| (1,1171) | 1:39:A:LEU:HD23 | 1:92:A:MET:HG2   | 10       | 1.27          |
| (1,1064) | 1:57:B:LYS:HD2  | 1:57:B:LYS:HB2   | 19       | 1.27          |
| (1,1063) | 1:57:A:LYS:HD2  | 1:57:A:LYS:HB2   | 19       | 1.27          |
| (1,1004) | 1:53:B:PHE:HB3  | 1:22:B:VAL:HG22  | 2        | 1.27          |
| (1,1004) | 1:53:B:PHE:HB3  | 1:22:B:VAL:HG22  | 20       | 1.27          |
| (1,1003) | 1:53:A:PHE:HB3  | 1:22:A:VAL:HG22  | 2        | 1.27          |
| (1,936)  | 1:98:B:ALA:HA   | 1:97:B:ALA:HB3   | 7        | 1.27          |
| (1,935)  | 1:98:A:ALA:HA   | 1:97:A:ALA:HB3   | 7        | 1.27          |
| (1,3053) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HG   | 2        | 1.26          |
| (1,2812) | 1:81:B:THR:H    | 1:79:B:TYR:HB2   | 3        | 1.26          |
| (1,2811) | 1:81:A:THR:H    | 1:79:A:TYR:HB2   | 3        | 1.26          |
| (1,1420) | 1:6:B:ILE:HG12  | 1:6:B:ILE:HG21   | 2        | 1.26          |
| (1,1420) | 1:6:B:ILE:HG12  | 1:6:B:ILE:HG23   | 4        | 1.26          |
| (1,1420) | 1:6:B:ILE:HG12  | 1:6:B:ILE:HG22   | 5        | 1.26          |
| (1,1420) | 1:6:B:ILE:HG12  | 1:6:B:ILE:HG21   | 8        | 1.26          |
| (1,1420) | 1:6:B:ILE:HG12  | 1:6:B:ILE:HG23   | 12       | 1.26          |
| (1,1419) | 1:6:A:ILE:HG12  | 1:6:A:ILE:HG21   | 2        | 1.26          |
| (1,1419) | 1:6:A:ILE:HG12  | 1:6:A:ILE:HG23   | 4        | 1.26          |
| (1,1419) | 1:6:A:ILE:HG12  | 1:6:A:ILE:HG22   | 5        | 1.26          |
| (1,1419) | 1:6:A:ILE:HG12  | 1:6:A:ILE:HG21   | 8        | 1.26          |
| (1,1419) | 1:6:A:ILE:HG12  | 1:6:A:ILE:HG22   | 20       | 1.26          |
| (1,1388) | 1:20:B:VAL:HG11 | 1:19:B:SER:H     | 14       | 1.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H     | 14       | 1.26          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 16       | 1.26          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 16       | 1.26          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG22  | 20       | 1.26          |
| (1,922)  | 1:116:B:ALA:HB1  | 1:115:B:LYS:HA   | 6        | 1.26          |
| (1,921)  | 1:116:A:ALA:HB1  | 1:115:A:LYS:HA   | 6        | 1.26          |
| (1,912)  | 1:9:B:ARG:HB2    | 1:6:B:ILE:HG13   | 1        | 1.26          |
| (1,911)  | 1:9:A:ARG:HB2    | 1:6:A:ILE:HG13   | 1        | 1.26          |
| (1,424)  | 1:87:B:VAL:HG11  | 1:53:B:PHE:HD1   | 13       | 1.26          |
| (1,423)  | 1:87:A:VAL:HG11  | 1:53:A:PHE:HD1   | 13       | 1.26          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 6        | 1.26          |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 6        | 1.26          |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG11  | 8        | 1.26          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG11  | 8        | 1.26          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 20       | 1.25          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 20       | 1.25          |
| (1,1419) | 1:6:A:ILE:HG12   | 1:6:A:ILE:HG23   | 12       | 1.25          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG13  | 6        | 1.25          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 7        | 1.25          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 7        | 1.25          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 6        | 1.25          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 13       | 1.25          |
| (1,180)  | 1:109:B:VAL:HG21 | 1:81:B:THR:HA    | 3        | 1.25          |
| (1,179)  | 1:109:A:VAL:HG21 | 1:81:A:THR:HA    | 3        | 1.25          |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 4        | 1.25          |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 4        | 1.25          |
| (1,3102) | 1:9:B:ARG:HB3    | 1:115:A:LYS:HA   | 2        | 1.24          |
| (1,3080) | 1:11:B:GLU:HG2   | 1:111:A:VAL:HG23 | 9        | 1.24          |
| (1,2608) | 1:107:B:ALA:H    | 1:56:B:THR:HG23  | 16       | 1.24          |
| (1,2607) | 1:107:A:ALA:H    | 1:56:A:THR:HG23  | 16       | 1.24          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG13  | 6        | 1.24          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG11  | 10       | 1.24          |
| (1,1332) | 1:64:B:VAL:HG23  | 1:65:B:ASP:HB3   | 19       | 1.24          |
| (1,1172) | 1:39:B:LEU:HD23  | 1:92:B:MET:HG2   | 13       | 1.24          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 6        | 1.24          |
| (1,543)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD22  | 17       | 1.24          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 13       | 1.24          |
| (1,3080) | 1:11:B:GLU:HG2   | 1:111:A:VAL:HG22 | 15       | 1.23          |
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG23 | 9        | 1.23          |
| (1,3075) | 1:42:A:VAL:HG23  | 1:99:B:TRP:HE1   | 19       | 1.23          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 16       | 1.23          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 16       | 1.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2160) | 1:77:B:ASN:H     | 1:115:B:LYS:HG2  | 8        | 1.23          |
| (1,2159) | 1:77:A:ASN:H     | 1:115:A:LYS:HG2  | 8        | 1.23          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 14       | 1.23          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 14       | 1.23          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 11       | 1.23          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 10       | 1.23          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 10       | 1.23          |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG12  | 15       | 1.23          |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG12  | 15       | 1.23          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG11  | 10       | 1.23          |
| (1,1331) | 1:64:A:VAL:HG23  | 1:65:A:ASP:HB3   | 19       | 1.23          |
| (1,1171) | 1:39:A:LEU:HD23  | 1:92:A:MET:HG2   | 13       | 1.23          |
| (1,544)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD22  | 17       | 1.23          |
| (1,180)  | 1:109:B:VAL:HG21 | 1:81:B:THR:HA    | 20       | 1.23          |
| (1,179)  | 1:109:A:VAL:HG21 | 1:81:A:THR:HA    | 20       | 1.23          |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG12  | 16       | 1.23          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG12  | 16       | 1.23          |
| (1,3076) | 1:42:B:VAL:HG21  | 1:99:A:TRP:HE1   | 15       | 1.22          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB3  | 18       | 1.22          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 13       | 1.22          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 8        | 1.22          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 13       | 1.22          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG22  | 14       | 1.22          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG22  | 14       | 1.22          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 11       | 1.22          |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG12  | 5        | 1.22          |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG12  | 5        | 1.22          |
| (1,1274) | 1:71:B:ILE:HD13  | 1:68:B:CYS:HB2   | 10       | 1.22          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 9        | 1.22          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 9        | 1.22          |
| (1,336)  | 1:36:B:VAL:HG11  | 1:30:B:ASP:HB2   | 11       | 1.22          |
| (1,335)  | 1:36:A:VAL:HG11  | 1:30:A:ASP:HB2   | 11       | 1.22          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 18       | 1.22          |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 18       | 1.22          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 8        | 1.21          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 8        | 1.21          |
| (1,1273) | 1:71:A:ILE:HD13  | 1:68:A:CYS:HB2   | 10       | 1.21          |
| (1,1130) | 1:77:B:ASN:HB2   | 1:113:B:SER:HB2  | 19       | 1.21          |
| (1,1129) | 1:77:A:ASN:HB2   | 1:113:A:SER:HB2  | 19       | 1.21          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 14       | 1.21          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 14       | 1.21          |
| (1,3076) | 1:42:B:VAL:HG23  | 1:99:A:TRP:HE1   | 19       | 1.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2556) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HB2  | 7        | 1.2           |
| (1,2551) | 1:76:A:TRP:HE1   | 1:75:A:HIS:HB2   | 11       | 1.2           |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 17       | 1.2           |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 3        | 1.2           |
| (1,2555) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HB2  | 7        | 1.19          |
| (1,2552) | 1:76:B:TRP:HE1   | 1:75:B:HIS:HB2   | 11       | 1.19          |
| (1,2280) | 1:25:B:LYS:H     | 1:22:B:VAL:HG23  | 17       | 1.19          |
| (1,2279) | 1:25:A:LYS:H     | 1:22:A:VAL:HG23  | 17       | 1.19          |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 17       | 1.19          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG21  | 11       | 1.19          |
| (1,922)  | 1:116:B:ALA:HB1  | 1:115:B:LYS:HA   | 4        | 1.19          |
| (1,921)  | 1:116:A:ALA:HB1  | 1:115:A:LYS:HA   | 4        | 1.19          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 5        | 1.19          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 5        | 1.19          |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 15       | 1.19          |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 15       | 1.19          |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 3        | 1.19          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 8        | 1.18          |
| (1,3075) | 1:42:A:VAL:HG21  | 1:99:B:TRP:HE1   | 15       | 1.18          |
| (1,1388) | 1:20:B:VAL:HG11  | 1:19:B:SER:H     | 1        | 1.18          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 7        | 1.18          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 7        | 1.18          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB3  | 19       | 1.18          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 14       | 1.17          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 14       | 1.17          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 15       | 1.17          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 15       | 1.17          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG21  | 11       | 1.17          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB3  | 19       | 1.17          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 10       | 1.17          |
| (1,336)  | 1:36:B:VAL:HG13  | 1:30:B:ASP:HB2   | 13       | 1.17          |
| (1,335)  | 1:36:A:VAL:HG13  | 1:30:A:ASP:HB2   | 13       | 1.17          |
| (1,251)  | 1:112:A:LEU:HD21 | 1:71:A:ILE:HA    | 4        | 1.17          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 1        | 1.16          |
| (1,3055) | 1:107:A:ALA:HB3  | 1:109:B:VAL:HG12 | 19       | 1.16          |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG23  | 9        | 1.16          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG23  | 9        | 1.16          |
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 14       | 1.16          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB2   | 20       | 1.16          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 20       | 1.16          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD21 | 17       | 1.16          |
| (1,1910) | 1:72:B:ASP:H     | 1:71:B:ILE:HG22  | 20       | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1909) | 1:72:A:ASP:H     | 1:71:A:ILE:HG22  | 20       | 1.16          |
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H     | 1        | 1.16          |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG21  | 6        | 1.16          |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG21  | 6        | 1.16          |
| (1,1172) | 1:39:B:LEU:HD21  | 1:92:B:MET:HG2   | 11       | 1.16          |
| (1,1171) | 1:39:A:LEU:HD21  | 1:92:A:MET:HG2   | 11       | 1.16          |
| (1,954)  | 1:18:B:VAL:HG23  | 1:59:B:ARG:HD2   | 6        | 1.16          |
| (1,953)  | 1:18:A:VAL:HG23  | 1:59:A:ARG:HD2   | 6        | 1.16          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 8        | 1.16          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA   | 8        | 1.16          |
| (1,840)  | 1:36:B:VAL:HG12  | 1:37:B:MET:HG3   | 19       | 1.16          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 10       | 1.16          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 11       | 1.16          |
| (1,252)  | 1:112:B:LEU:HD21 | 1:71:B:ILE:HA    | 4        | 1.16          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 20       | 1.15          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 19       | 1.15          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 20       | 1.15          |
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 20       | 1.15          |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 14       | 1.15          |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 20       | 1.15          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD21 | 17       | 1.15          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 12       | 1.15          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 12       | 1.15          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 16       | 1.15          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 16       | 1.15          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 17       | 1.15          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 17       | 1.15          |
| (1,839)  | 1:36:A:VAL:HG12  | 1:37:A:MET:HG3   | 19       | 1.15          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 17       | 1.15          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 17       | 1.15          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 11       | 1.15          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 1        | 1.14          |
| (1,3056) | 1:107:B:ALA:HB3  | 1:109:A:VAL:HG12 | 3        | 1.14          |
| (1,3055) | 1:107:A:ALA:HB3  | 1:109:B:VAL:HG12 | 3        | 1.14          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 19       | 1.14          |
| (1,1873) | 1:21:A:TRP:H     | 1:21:A:TRP:HE3   | 11       | 1.14          |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG13  | 4        | 1.14          |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG13  | 4        | 1.14          |
| (1,1388) | 1:20:B:VAL:HG12  | 1:19:B:SER:H     | 8        | 1.14          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 10       | 1.14          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 10       | 1.14          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG23  | 6        | 1.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,440)  | 1:88:B:LYS:HA   | 1:88:B:LYS:HE2   | 1        | 1.14          |
| (1,439)  | 1:88:A:LYS:HA   | 1:88:A:LYS:HE2   | 1        | 1.14          |
| (1,96)   | 1:22:B:VAL:HG13 | 1:53:B:PHE:HB3   | 12       | 1.14          |
| (1,95)   | 1:22:A:VAL:HG13 | 1:53:A:PHE:HB3   | 12       | 1.14          |
| (1,1874) | 1:21:B:TRP:H    | 1:21:B:TRP:HE3   | 11       | 1.13          |
| (1,1004) | 1:53:B:PHE:HB3  | 1:22:B:VAL:HG23  | 6        | 1.13          |
| (1,818)  | 1:31:B:ILE:HG21 | 1:32:B:LYS:HG2   | 4        | 1.13          |
| (1,817)  | 1:31:A:ILE:HG21 | 1:32:A:LYS:HG2   | 4        | 1.13          |
| (1,668)  | 1:42:B:VAL:HG13 | 1:99:B:TRP:HZ2   | 20       | 1.13          |
| (1,667)  | 1:42:A:VAL:HG13 | 1:99:A:TRP:HZ2   | 20       | 1.13          |
| (1,542)  | 1:92:B:MET:HE2  | 1:39:B:LEU:HD11  | 1        | 1.13          |
| (1,226)  | 1:63:B:PRO:HB3  | 1:64:B:VAL:HG21  | 8        | 1.13          |
| (1,225)  | 1:63:A:PRO:HB3  | 1:64:A:VAL:HG21  | 8        | 1.13          |
| (1,3076) | 1:42:B:VAL:HG21 | 1:99:A:TRP:HE1   | 11       | 1.12          |
| (1,3075) | 1:42:A:VAL:HG21 | 1:99:B:TRP:HE1   | 11       | 1.12          |
| (1,3064) | 1:12:B:PHE:H    | 1:111:A:VAL:HG13 | 6        | 1.12          |
| (1,3060) | 1:71:B:ILE:HD13 | 1:14:A:VAL:HB    | 2        | 1.12          |
| (1,3060) | 1:71:B:ILE:HD12 | 1:14:A:VAL:HB    | 3        | 1.12          |
| (1,2812) | 1:81:B:THR:H    | 1:79:B:TYR:HB2   | 13       | 1.12          |
| (1,2811) | 1:81:A:THR:H    | 1:79:A:TYR:HB2   | 13       | 1.12          |
| (1,1996) | 1:67:B:GLY:H    | 1:64:B:VAL:HB    | 3        | 1.12          |
| (1,1387) | 1:20:A:VAL:HG12 | 1:19:A:SER:H     | 8        | 1.12          |
| (1,1320) | 1:34:B:LYS:HD2  | 1:34:B:LYS:HB3   | 3        | 1.12          |
| (1,1320) | 1:34:B:LYS:HD2  | 1:34:B:LYS:HB3   | 20       | 1.12          |
| (1,1319) | 1:34:A:LYS:HD2  | 1:34:A:LYS:HB3   | 3        | 1.12          |
| (1,1319) | 1:34:A:LYS:HD2  | 1:34:A:LYS:HB3   | 20       | 1.12          |
| (1,1130) | 1:77:B:ASN:HB2  | 1:113:B:SER:HB2  | 11       | 1.12          |
| (1,1129) | 1:77:A:ASN:HB2  | 1:113:A:SER:HB2  | 11       | 1.12          |
| (1,920)  | 1:117:B:VAL:HB  | 1:116:B:ALA:HB3  | 8        | 1.12          |
| (1,919)  | 1:117:A:VAL:HB  | 1:116:A:ALA:HB3  | 8        | 1.12          |
| (1,541)  | 1:92:A:MET:HE2  | 1:39:A:LEU:HD11  | 1        | 1.12          |
| (1,96)   | 1:22:B:VAL:HG12 | 1:53:B:PHE:HB3   | 19       | 1.12          |
| (1,95)   | 1:22:A:VAL:HG12 | 1:53:A:PHE:HB3   | 19       | 1.12          |
| (1,3056) | 1:107:B:ALA:HB3 | 1:109:A:VAL:HG12 | 19       | 1.11          |
| (1,1995) | 1:67:A:GLY:H    | 1:64:A:VAL:HB    | 3        | 1.11          |
| (1,1320) | 1:34:B:LYS:HD2  | 1:34:B:LYS:HB3   | 2        | 1.11          |
| (1,1320) | 1:34:B:LYS:HD2  | 1:34:B:LYS:HB3   | 17       | 1.11          |
| (1,1319) | 1:34:A:LYS:HD2  | 1:34:A:LYS:HB3   | 2        | 1.11          |
| (1,1319) | 1:34:A:LYS:HD2  | 1:34:A:LYS:HB3   | 17       | 1.11          |
| (1,912)  | 1:9:B:ARG:HB2   | 1:6:B:ILE:HG13   | 14       | 1.11          |
| (1,911)  | 1:9:A:ARG:HB2   | 1:6:A:ILE:HG13   | 14       | 1.11          |
| (1,818)  | 1:31:B:ILE:HG22 | 1:32:B:LYS:HG2   | 7        | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,544)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD22  | 6        | 1.11          |
| (1,543)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD22  | 6        | 1.11          |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA    | 5        | 1.1           |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 5        | 1.1           |
| (1,3059) | 1:71:A:ILE:HD12  | 1:14:B:VAL:HB    | 3        | 1.1           |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG22  | 3        | 1.1           |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG22  | 3        | 1.1           |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 2        | 1.1           |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 2        | 1.1           |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB3   | 11       | 1.1           |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB3   | 11       | 1.1           |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 5        | 1.1           |
| (1,817)  | 1:31:A:ILE:HG22  | 1:32:A:LYS:HG2   | 7        | 1.1           |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 9        | 1.1           |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 9        | 1.1           |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB3   | 5        | 1.1           |
| (1,544)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD23  | 2        | 1.1           |
| (1,543)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD23  | 2        | 1.1           |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 16       | 1.1           |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 16       | 1.1           |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG12  | 3        | 1.1           |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB3   | 5        | 1.09          |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB3   | 5        | 1.09          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 5        | 1.09          |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB3   | 5        | 1.09          |
| (1,541)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD12  | 10       | 1.09          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG12  | 3        | 1.09          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB3  | 17       | 1.08          |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG13 | 6        | 1.08          |
| (1,3059) | 1:71:A:ILE:HD13  | 1:14:B:VAL:HB    | 2        | 1.08          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG23  | 2        | 1.08          |
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 18       | 1.08          |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 18       | 1.08          |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB3   | 6        | 1.08          |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB3   | 6        | 1.08          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG22  | 7        | 1.08          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 19       | 1.08          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 19       | 1.08          |
| (1,542)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD12  | 10       | 1.08          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 18       | 1.08          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB3  | 17       | 1.07          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD13  | 12       | 1.07          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG23  | 2        | 1.07          |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG11  | 10       | 1.07          |
| (1,2501) | 1:69:A:ARG:H     | 1:64:A:VAL:HG11  | 10       | 1.07          |
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 13       | 1.07          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB1   | 15       | 1.07          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD23 | 4        | 1.07          |
| (1,1543) | 1:55:A:GLU:HG3   | 1:20:A:VAL:HG23  | 6        | 1.07          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 13       | 1.07          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 13       | 1.07          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 7        | 1.07          |
| (1,1247) | 1:71:A:ILE:HG12  | 1:70:A:GLY:HA3   | 7        | 1.07          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG22  | 7        | 1.07          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG12  | 11       | 1.07          |
| (1,270)  | 1:14:B:VAL:HG11  | 1:110:B:CYS:HB3  | 14       | 1.07          |
| (1,269)  | 1:14:A:VAL:HG11  | 1:110:A:CYS:HB3  | 14       | 1.07          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 18       | 1.07          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG21  | 7        | 1.07          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG21  | 7        | 1.07          |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD13  | 12       | 1.06          |
| (1,2545) | 1:72:A:ASP:H     | 1:76:A:TRP:HE1   | 5        | 1.06          |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 13       | 1.06          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB1   | 15       | 1.06          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD23 | 4        | 1.06          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD22 | 5        | 1.06          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD22 | 5        | 1.06          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 3        | 1.06          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 3        | 1.06          |
| (1,1544) | 1:55:B:GLU:HG3   | 1:20:B:VAL:HG23  | 6        | 1.06          |
| (1,1119) | 1:64:A:VAL:HG22  | 1:65:A:ASP:HB2   | 20       | 1.06          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 8        | 1.06          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 8        | 1.06          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG12  | 11       | 1.06          |
| (1,3081) | 1:12:A:PHE:H     | 1:111:B:VAL:HG21 | 19       | 1.05          |
| (1,2546) | 1:72:B:ASP:H     | 1:76:B:TRP:HE1   | 5        | 1.05          |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG11  | 3        | 1.05          |
| (1,2501) | 1:69:A:ARG:H     | 1:64:A:VAL:HG11  | 3        | 1.05          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB2   | 2        | 1.05          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 2        | 1.05          |
| (1,1818) | 1:114:B:ARG:H    | 1:76:B:TRP:HE3   | 17       | 1.05          |
| (1,1817) | 1:114:A:ARG:H    | 1:76:A:TRP:HE3   | 17       | 1.05          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 15       | 1.05          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 9        | 1.05          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1120) | 1:64:B:VAL:HG22  | 1:65:B:ASP:HB2   | 20       | 1.05          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 5        | 1.05          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA   | 5        | 1.05          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB3  | 13       | 1.05          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB3  | 13       | 1.05          |
| (1,840)  | 1:36:B:VAL:HG12  | 1:37:B:MET:HG3   | 3        | 1.05          |
| (1,840)  | 1:36:B:VAL:HG12  | 1:37:B:MET:HG3   | 15       | 1.05          |
| (1,839)  | 1:36:A:VAL:HG12  | 1:37:A:MET:HG3   | 3        | 1.05          |
| (1,839)  | 1:36:A:VAL:HG12  | 1:37:A:MET:HG3   | 15       | 1.05          |
| (1,550)  | 1:92:B:MET:HE3   | 1:97:B:ALA:HB3   | 14       | 1.05          |
| (1,549)  | 1:92:A:MET:HE3   | 1:97:A:ALA:HB3   | 14       | 1.05          |
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG22  | 1        | 1.05          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG22  | 1        | 1.05          |
| (1,225)  | 1:63:A:PRO:HB3   | 1:64:A:VAL:HG22  | 3        | 1.05          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 12       | 1.04          |
| (1,3082) | 1:12:B:PHE:H     | 1:111:A:VAL:HG21 | 19       | 1.04          |
| (1,1886) | 1:21:B:TRP:H     | 1:54:B:PHE:HD1   | 10       | 1.04          |
| (1,1885) | 1:21:A:TRP:H     | 1:54:A:PHE:HD1   | 10       | 1.04          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 9        | 1.04          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 18       | 1.04          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 15       | 1.04          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 18       | 1.04          |
| (1,922)  | 1:116:B:ALA:HB1  | 1:115:B:LYS:HA   | 14       | 1.04          |
| (1,921)  | 1:116:A:ALA:HB1  | 1:115:A:LYS:HA   | 14       | 1.04          |
| (1,818)  | 1:31:B:ILE:HG23  | 1:32:B:LYS:HG2   | 8        | 1.04          |
| (1,817)  | 1:31:A:ILE:HG23  | 1:32:A:LYS:HG2   | 8        | 1.04          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 7        | 1.04          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 7        | 1.04          |
| (1,288)  | 1:106:B:THR:HG23 | 1:85:B:THR:HG23  | 16       | 1.04          |
| (1,226)  | 1:63:B:PRO:HB3   | 1:64:B:VAL:HG22  | 3        | 1.04          |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG13  | 10       | 1.04          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG13  | 10       | 1.04          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD23 | 1        | 1.03          |
| (1,3061) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HD13 | 7        | 1.03          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB3   | 19       | 1.03          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB3   | 19       | 1.03          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 6        | 1.03          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 6        | 1.03          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 8        | 1.03          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG23  | 19       | 1.03          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 20       | 1.03          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 8        | 1.03          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 7        | 1.03          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 7        | 1.03          |
| (1,287)  | 1:106:A:THR:HG23 | 1:85:A:THR:HG23  | 16       | 1.03          |
| (1,180)  | 1:109:B:VAL:HG22 | 1:81:B:THR:HA    | 10       | 1.03          |
| (3,2)    | 1:52:B:TYR:HB2   | 1:51:B:GLN:HG3   | 18       | 1.02          |
| (3,1)    | 1:52:A:TYR:HB2   | 1:51:A:GLN:HG3   | 18       | 1.02          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 12       | 1.02          |
| (1,3081) | 1:12:A:PHE:H     | 1:111:B:VAL:HG22 | 11       | 1.02          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 3        | 1.02          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 3        | 1.02          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 20       | 1.02          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 15       | 1.02          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 15       | 1.02          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG23  | 19       | 1.02          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 20       | 1.02          |
| (1,1120) | 1:64:B:VAL:HG23  | 1:65:B:ASP:HB2   | 19       | 1.02          |
| (1,1119) | 1:64:A:VAL:HG23  | 1:65:A:ASP:HB2   | 19       | 1.02          |
| (1,257)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HB2   | 20       | 1.02          |
| (1,179)  | 1:109:A:VAL:HG22 | 1:81:A:THR:HA    | 10       | 1.02          |
| (1,3062) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HD13 | 7        | 1.01          |
| (1,2280) | 1:25:B:LYS:H     | 1:22:B:VAL:HG23  | 4        | 1.01          |
| (1,2279) | 1:25:A:LYS:H     | 1:22:A:VAL:HG23  | 4        | 1.01          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 20       | 1.01          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 6        | 1.01          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 15       | 1.01          |
| (1,954)  | 1:18:B:VAL:HG22  | 1:59:B:ARG:HD2   | 20       | 1.01          |
| (1,953)  | 1:18:A:VAL:HG22  | 1:59:A:ARG:HD2   | 20       | 1.01          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 19       | 1.01          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA   | 19       | 1.01          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 7        | 1.01          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 7        | 1.01          |
| (1,288)  | 1:106:B:THR:HG23 | 1:85:B:THR:HG21  | 9        | 1.01          |
| (1,258)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HB2   | 20       | 1.01          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD23 | 1        | 1.0           |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD23 | 17       | 1.0           |
| (1,3072) | 1:44:B:ILE:HD13  | 1:99:A:TRP:HE1   | 12       | 1.0           |
| (1,2159) | 1:77:A:ASN:H     | 1:115:A:LYS:HG2  | 7        | 1.0           |
| (1,1926) | 1:72:B:ASP:H     | 1:71:B:ILE:HD13  | 5        | 1.0           |
| (1,1925) | 1:72:A:ASP:H     | 1:71:A:ILE:HD13  | 5        | 1.0           |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 6        | 1.0           |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 12       | 1.0           |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 12       | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 1        | 1.0           |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 15       | 1.0           |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21  | 10       | 1.0           |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21  | 10       | 1.0           |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB2   | 15       | 1.0           |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB2   | 15       | 1.0           |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG13 | 13       | 1.0           |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG13 | 13       | 1.0           |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB2  | 15       | 1.0           |
| (1,840)  | 1:36:B:VAL:HG11  | 1:37:B:MET:HG3   | 7        | 1.0           |
| (1,840)  | 1:36:B:VAL:HG11  | 1:37:B:MET:HG3   | 16       | 1.0           |
| (1,839)  | 1:36:A:VAL:HG11  | 1:37:A:MET:HG3   | 16       | 1.0           |
| (1,336)  | 1:36:B:VAL:HG13  | 1:30:B:ASP:HB2   | 19       | 1.0           |
| (1,287)  | 1:106:A:THR:HG23 | 1:85:A:THR:HG21  | 9        | 1.0           |
| (1,270)  | 1:14:B:VAL:HG12  | 1:110:B:CYS:HB3  | 3        | 1.0           |
| (1,269)  | 1:14:A:VAL:HG12  | 1:110:A:CYS:HB3  | 3        | 1.0           |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 2        | 1.0           |
| (1,3082) | 1:12:B:PHE:H     | 1:111:A:VAL:HG22 | 11       | 0.99          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG21  | 14       | 0.99          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 16       | 0.99          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 16       | 0.99          |
| (1,2160) | 1:77:B:ASN:H     | 1:115:B:LYS:HG2  | 7        | 0.99          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 17       | 0.99          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 1        | 0.99          |
| (1,1172) | 1:39:B:LEU:HD21  | 1:92:B:MET:HG2   | 3        | 0.99          |
| (1,1171) | 1:39:A:LEU:HD21  | 1:92:A:MET:HG2   | 3        | 0.99          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA   | 2        | 0.99          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB2  | 15       | 0.99          |
| (1,839)  | 1:36:A:VAL:HG11  | 1:37:A:MET:HG3   | 7        | 0.99          |
| (1,598)  | 1:107:B:ALA:HB1  | 1:83:B:THR:HA    | 16       | 0.99          |
| (1,597)  | 1:107:A:ALA:HB1  | 1:83:A:THR:HA    | 16       | 0.99          |
| (1,335)  | 1:36:A:VAL:HG13  | 1:30:A:ASP:HB2   | 19       | 0.99          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 2        | 0.99          |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA    | 5        | 0.99          |
| (1,3071) | 1:44:A:ILE:HD13  | 1:99:B:TRP:HE1   | 12       | 0.98          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD11  | 3        | 0.98          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG21  | 14       | 0.98          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 19       | 0.98          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 19       | 0.98          |
| (1,2380) | 1:29:B:THR:H     | 1:103:B:ARG:HB2  | 2        | 0.98          |
| (1,2379) | 1:29:A:THR:H     | 1:103:A:ARG:HB2  | 2        | 0.98          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 13       | 0.98          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1388) | 1:20:B:VAL:HG11  | 1:19:B:SER:H     | 5        | 0.98          |
| (1,1314) | 1:70:B:GLY:H     | 1:64:B:VAL:HG11  | 16       | 0.98          |
| (1,1313) | 1:70:A:GLY:H     | 1:64:A:VAL:HG11  | 16       | 0.98          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 5        | 0.98          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 2        | 0.98          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 3        | 0.98          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA   | 3        | 0.98          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 1        | 0.98          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 15       | 0.98          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 1        | 0.98          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 15       | 0.98          |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 4        | 0.98          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 4        | 0.98          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 6        | 0.98          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 6        | 0.98          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 5        | 0.98          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD23 | 17       | 0.97          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 8        | 0.97          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG21  | 11       | 0.97          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG11 | 12       | 0.97          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG11 | 12       | 0.97          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 13       | 0.97          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 17       | 0.97          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 19       | 0.97          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 19       | 0.97          |
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H     | 5        | 0.97          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 14       | 0.97          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 14       | 0.97          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG23  | 13       | 0.97          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG23  | 13       | 0.97          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 5        | 0.97          |
| (1,912)  | 1:9:B:ARG:HB2    | 1:6:B:ILE:HG13   | 2        | 0.97          |
| (1,911)  | 1:9:A:ARG:HB2    | 1:6:A:ILE:HG13   | 2        | 0.97          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 3        | 0.97          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 13       | 0.97          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 18       | 0.97          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 3        | 0.97          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 13       | 0.97          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 18       | 0.97          |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 19       | 0.97          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 19       | 0.97          |
| (1,288)  | 1:106:B:THR:HG23 | 1:85:B:THR:HG21  | 7        | 0.97          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,287)  | 1:106:A:THR:HG23 | 1:85:A:THR:HG21 | 7        | 0.97          |
| (1,270)  | 1:14:B:VAL:HG11  | 1:110:B:CYS:HB3 | 2        | 0.97          |
| (1,269)  | 1:14:A:VAL:HG11  | 1:110:A:CYS:HB3 | 2        | 0.97          |
| (1,3088) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HA   | 11       | 0.96          |
| (1,3087) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HA   | 11       | 0.96          |
| (1,3052) | 1:21:B:TRP:HE1   | 1:31:A:ILE:HD13 | 2        | 0.96          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3  | 8        | 0.96          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG21 | 11       | 0.96          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21 | 14       | 0.96          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21 | 14       | 0.96          |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2  | 10       | 0.96          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2  | 10       | 0.96          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2  | 18       | 0.96          |
| (1,3086) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HG22 | 11       | 0.95          |
| (1,3085) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HG22 | 11       | 0.95          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB3 | 4        | 0.95          |
| (1,3059) | 1:71:A:ILE:HD12  | 1:14:B:VAL:HB   | 1        | 0.95          |
| (1,3051) | 1:21:A:TRP:HE1   | 1:31:B:ILE:HD13 | 2        | 0.95          |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD11 | 3        | 0.95          |
| (1,2298) | 1:98:B:ALA:H     | 1:97:B:ALA:HB3  | 7        | 0.95          |
| (1,1996) | 1:67:B:GLY:H     | 1:64:B:VAL:HB   | 7        | 0.95          |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB3  | 3        | 0.95          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3  | 4        | 0.95          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3  | 11       | 0.95          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3  | 4        | 0.95          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3  | 11       | 0.95          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB   | 10       | 0.95          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB   | 10       | 0.95          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG23 | 16       | 0.95          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG23 | 16       | 0.95          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1  | 14       | 0.95          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1  | 14       | 0.95          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA  | 16       | 0.95          |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2  | 18       | 0.95          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3  | 10       | 0.95          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2  | 18       | 0.95          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2  | 17       | 0.95          |
| (1,52)   | 1:42:B:VAL:HG23  | 1:42:B:VAL:HG13 | 2        | 0.95          |
| (1,51)   | 1:42:A:VAL:HG23  | 1:42:A:VAL:HG13 | 2        | 0.95          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3  | 4        | 0.94          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3  | 4        | 0.94          |
| (1,2298) | 1:98:B:ALA:H     | 1:97:B:ALA:HB1  | 9        | 0.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2297) | 1:98:A:ALA:H     | 1:97:A:ALA:HB3   | 7        | 0.94          |
| (1,1995) | 1:67:A:GLY:H     | 1:64:A:VAL:HB    | 7        | 0.94          |
| (1,1436) | 1:38:B:VAL:HG21  | 1:28:B:ALA:HB3   | 5        | 0.94          |
| (1,1435) | 1:38:A:VAL:HG21  | 1:28:A:ALA:HB3   | 5        | 0.94          |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB3   | 3        | 0.94          |
| (1,1172) | 1:39:B:LEU:HD23  | 1:92:B:MET:HG2   | 4        | 0.94          |
| (1,952)  | 1:115:B:LYS:H    | 1:76:B:TRP:HA    | 8        | 0.94          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 16       | 0.94          |
| (1,908)  | 1:5:B:PRO:HA     | 1:9:B:ARG:HB2    | 9        | 0.94          |
| (1,907)  | 1:5:A:PRO:HA     | 1:9:A:ARG:HB2    | 9        | 0.94          |
| (1,668)  | 1:42:B:VAL:HG12  | 1:99:B:TRP:HZ2   | 19       | 0.94          |
| (1,667)  | 1:42:A:VAL:HG12  | 1:99:A:TRP:HZ2   | 19       | 0.94          |
| (1,548)  | 1:92:B:MET:HE3   | 1:92:B:MET:HB2   | 9        | 0.94          |
| (1,547)  | 1:92:A:MET:HE3   | 1:92:A:MET:HB2   | 9        | 0.94          |
| (1,547)  | 1:92:A:MET:HE3   | 1:92:A:MET:HB2   | 18       | 0.94          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 10       | 0.94          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 17       | 0.94          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 5        | 0.94          |
| (1,100)  | 1:22:B:VAL:HG11  | 1:55:B:GLU:HB2   | 5        | 0.94          |
| (1,96)   | 1:22:B:VAL:HG11  | 1:53:B:PHE:HB3   | 1        | 0.94          |
| (1,3082) | 1:12:B:PHE:H     | 1:111:A:VAL:HG22 | 7        | 0.93          |
| (1,3060) | 1:71:B:ILE:HD12  | 1:14:A:VAL:HB    | 1        | 0.93          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 1        | 0.93          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 1        | 0.93          |
| (1,2297) | 1:98:A:ALA:H     | 1:97:A:ALA:HB1   | 9        | 0.93          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 9        | 0.93          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 9        | 0.93          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 5        | 0.93          |
| (1,1449) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HE1   | 5        | 0.93          |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB3   | 8        | 0.93          |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB3   | 8        | 0.93          |
| (1,1388) | 1:20:B:VAL:HG11  | 1:19:B:SER:H     | 10       | 0.93          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG23  | 13       | 0.93          |
| (1,1171) | 1:39:A:LEU:HD23  | 1:92:A:MET:HG2   | 4        | 0.93          |
| (1,951)  | 1:115:A:LYS:H    | 1:76:A:TRP:HA    | 8        | 0.93          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB3   | 10       | 0.93          |
| (1,840)  | 1:36:B:VAL:HG12  | 1:37:B:MET:HG3   | 9        | 0.93          |
| (1,839)  | 1:36:A:VAL:HG12  | 1:37:A:MET:HG3   | 9        | 0.93          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 5        | 0.93          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 5        | 0.93          |
| (1,548)  | 1:92:B:MET:HE1   | 1:92:B:MET:HB2   | 12       | 0.93          |
| (1,547)  | 1:92:A:MET:HE1   | 1:92:A:MET:HB2   | 12       | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 5        | 0.93          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG23  | 3        | 0.93          |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG23  | 3        | 0.93          |
| (1,99)   | 1:22:A:VAL:HG11  | 1:55:A:GLU:HB2   | 5        | 0.93          |
| (1,95)   | 1:22:A:VAL:HG11  | 1:53:A:PHE:HB3   | 1        | 0.93          |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG12  | 17       | 0.93          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG12  | 17       | 0.93          |
| (1,52)   | 1:42:B:VAL:HG23  | 1:42:B:VAL:HG13  | 6        | 0.93          |
| (1,51)   | 1:42:A:VAL:HG23  | 1:42:A:VAL:HG13  | 6        | 0.93          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 13       | 0.92          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 15       | 0.92          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 15       | 0.92          |
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H     | 10       | 0.92          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG23  | 13       | 0.92          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 11       | 0.92          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB3   | 10       | 0.92          |
| (1,839)  | 1:36:A:VAL:HG13  | 1:37:A:MET:HG3   | 11       | 0.92          |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2   | 14       | 0.92          |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 15       | 0.92          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 15       | 0.92          |
| (1,52)   | 1:42:B:VAL:HG23  | 1:42:B:VAL:HG11  | 13       | 0.92          |
| (1,51)   | 1:42:A:VAL:HG23  | 1:42:A:VAL:HG12  | 7        | 0.92          |
| (1,51)   | 1:42:A:VAL:HG23  | 1:42:A:VAL:HG11  | 13       | 0.92          |
| (1,3081) | 1:12:A:PHE:H     | 1:111:B:VAL:HG22 | 7        | 0.91          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB3  | 4        | 0.91          |
| (1,3067) | 1:70:A:GLY:HA3   | 1:71:B:ILE:HG21  | 16       | 0.91          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 1        | 0.91          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 1        | 0.91          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 8        | 0.91          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 3        | 0.91          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 3        | 0.91          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB2   | 6        | 0.91          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB2   | 6        | 0.91          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 11       | 0.91          |
| (1,840)  | 1:36:B:VAL:HG13  | 1:37:B:MET:HG3   | 11       | 0.91          |
| (1,818)  | 1:31:B:ILE:HG22  | 1:32:B:LYS:HG2   | 2        | 0.91          |
| (1,817)  | 1:31:A:ILE:HG22  | 1:32:A:LYS:HG2   | 2        | 0.91          |
| (1,548)  | 1:92:B:MET:HE1   | 1:92:B:MET:HB2   | 6        | 0.91          |
| (1,547)  | 1:92:A:MET:HE1   | 1:92:A:MET:HB2   | 6        | 0.91          |
| (1,547)  | 1:92:A:MET:HE3   | 1:92:A:MET:HB2   | 7        | 0.91          |
| (1,547)  | 1:92:A:MET:HE2   | 1:92:A:MET:HB2   | 14       | 0.91          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG22  | 3        | 0.91          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,428)  | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG23  | 20       | 0.91          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG22  | 3        | 0.91          |
| (1,427)  | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG23  | 20       | 0.91          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG23  | 11       | 0.91          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG23  | 11       | 0.91          |
| (1,344)  | 1:48:B:VAL:HG12  | 1:41:B:GLU:HG2   | 20       | 0.91          |
| (1,343)  | 1:48:A:VAL:HG12  | 1:41:A:GLU:HG2   | 20       | 0.91          |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG11  | 1        | 0.91          |
| (1,52)   | 1:42:B:VAL:HG23  | 1:42:B:VAL:HG12  | 7        | 0.91          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG11  | 1        | 0.91          |
| (1,3068) | 1:70:B:GLY:HA3   | 1:71:A:ILE:HG21  | 16       | 0.9           |
| (1,3056) | 1:107:B:ALA:HB2  | 1:109:A:VAL:HG11 | 9        | 0.9           |
| (1,3055) | 1:107:A:ALA:HB2  | 1:109:B:VAL:HG11 | 9        | 0.9           |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG21  | 10       | 0.9           |
| (1,2501) | 1:69:A:ARG:H     | 1:64:A:VAL:HG12  | 7        | 0.9           |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 4        | 0.9           |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 4        | 0.9           |
| (1,2256) | 1:77:B:ASN:HD22  | 1:115:B:LYS:HG2  | 19       | 0.9           |
| (1,2255) | 1:77:A:ASN:HD22  | 1:115:A:LYS:HG2  | 19       | 0.9           |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB1   | 17       | 0.9           |
| (1,2074) | 1:88:B:LYS:H     | 1:88:B:LYS:HB2   | 11       | 0.9           |
| (1,2073) | 1:88:A:LYS:H     | 1:88:A:LYS:HB2   | 11       | 0.9           |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 8        | 0.9           |
| (1,1216) | 1:22:B:VAL:HG11  | 1:20:B:VAL:HB    | 1        | 0.9           |
| (1,1215) | 1:22:A:VAL:HG11  | 1:20:A:VAL:HB    | 1        | 0.9           |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG23  | 2        | 0.9           |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG22  | 9        | 0.9           |
| (1,840)  | 1:36:B:VAL:HG12  | 1:37:B:MET:HG3   | 1        | 0.9           |
| (1,839)  | 1:36:A:VAL:HG12  | 1:37:A:MET:HG3   | 1        | 0.9           |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2   | 2        | 0.9           |
| (1,548)  | 1:92:B:MET:HE3   | 1:92:B:MET:HB2   | 7        | 0.9           |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2   | 11       | 0.9           |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2   | 16       | 0.9           |
| (1,548)  | 1:92:B:MET:HE3   | 1:92:B:MET:HB2   | 17       | 0.9           |
| (1,547)  | 1:92:A:MET:HE2   | 1:92:A:MET:HB2   | 2        | 0.9           |
| (1,547)  | 1:92:A:MET:HE1   | 1:92:A:MET:HB2   | 4        | 0.9           |
| (1,547)  | 1:92:A:MET:HE2   | 1:92:A:MET:HB2   | 11       | 0.9           |
| (1,547)  | 1:92:A:MET:HE2   | 1:92:A:MET:HB2   | 16       | 0.9           |
| (1,547)  | 1:92:A:MET:HE3   | 1:92:A:MET:HB2   | 17       | 0.9           |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG21  | 2        | 0.9           |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG21  | 2        | 0.9           |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG21  | 20       | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,356)  | 1:41:B:GLU:HG2   | 1:48:B:VAL:HA    | 7        | 0.9           |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG11  | 9        | 0.9           |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG13  | 10       | 0.9           |
| (1,52)   | 1:42:B:VAL:HG21  | 1:42:B:VAL:HG11  | 18       | 0.9           |
| (1,51)   | 1:42:A:VAL:HG21  | 1:42:A:VAL:HG13  | 8        | 0.9           |
| (1,51)   | 1:42:A:VAL:HG21  | 1:42:A:VAL:HG11  | 18       | 0.9           |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG21  | 10       | 0.89          |
| (1,2552) | 1:76:B:TRP:HE1   | 1:75:B:HIS:HB2   | 5        | 0.89          |
| (1,2551) | 1:76:A:TRP:HE1   | 1:75:A:HIS:HB2   | 5        | 0.89          |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG12  | 7        | 0.89          |
| (1,2348) | 1:85:B:THR:H     | 1:106:B:THR:HG21 | 16       | 0.89          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB1   | 17       | 0.89          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 17       | 0.89          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 17       | 0.89          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 9        | 0.89          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 9        | 0.89          |
| (1,1320) | 1:34:B:LYS:HD2   | 1:34:B:LYS:HB3   | 19       | 0.89          |
| (1,1319) | 1:34:A:LYS:HD2   | 1:34:A:LYS:HB3   | 19       | 0.89          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG23  | 2        | 0.89          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG22  | 9        | 0.89          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG22  | 15       | 0.89          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG22  | 15       | 0.89          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 2        | 0.89          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB3   | 4        | 0.89          |
| (1,548)  | 1:92:B:MET:HE1   | 1:92:B:MET:HB2   | 4        | 0.89          |
| (1,544)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD23  | 7        | 0.89          |
| (1,543)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD23  | 7        | 0.89          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 9        | 0.89          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 2        | 0.89          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 2        | 0.89          |
| (1,428)  | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG22  | 13       | 0.89          |
| (1,428)  | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG22  | 14       | 0.89          |
| (1,428)  | 1:87:B:VAL:HG13  | 1:87:B:VAL:HG23  | 17       | 0.89          |
| (1,427)  | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG22  | 13       | 0.89          |
| (1,427)  | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG22  | 14       | 0.89          |
| (1,427)  | 1:87:A:VAL:HG13  | 1:87:A:VAL:HG23  | 17       | 0.89          |
| (1,427)  | 1:87:A:VAL:HG13  | 1:87:A:VAL:HG23  | 19       | 0.89          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG22  | 16       | 0.89          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG21  | 20       | 0.89          |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG22  | 16       | 0.89          |
| (1,355)  | 1:41:A:GLU:HG2   | 1:48:A:VAL:HA    | 7        | 0.89          |
| (1,288)  | 1:106:B:THR:HG21 | 1:85:B:THR:HG22  | 8        | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,287)  | 1:106:A:THR:HG21 | 1:85:A:THR:HG22  | 8        | 0.89          |
| (1,52)   | 1:42:B:VAL:HG23  | 1:42:B:VAL:HG12  | 4        | 0.89          |
| (1,52)   | 1:42:B:VAL:HG21  | 1:42:B:VAL:HG13  | 8        | 0.89          |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG13  | 17       | 0.89          |
| (1,51)   | 1:42:A:VAL:HG21  | 1:42:A:VAL:HG11  | 5        | 0.89          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG11  | 9        | 0.89          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG13  | 10       | 0.89          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG12  | 16       | 0.89          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG13  | 17       | 0.89          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 7        | 0.88          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 16       | 0.88          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 16       | 0.88          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG23  | 5        | 0.88          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG23  | 20       | 0.88          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG23  | 5        | 0.88          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG23  | 20       | 0.88          |
| (1,2347) | 1:85:A:THR:H     | 1:106:A:THR:HG21 | 16       | 0.88          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG13 | 19       | 0.88          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB2   | 14       | 0.88          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 14       | 0.88          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 20       | 0.88          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 20       | 0.88          |
| (1,1910) | 1:72:B:ASP:H     | 1:71:B:ILE:HG23  | 6        | 0.88          |
| (1,1909) | 1:72:A:ASP:H     | 1:71:A:ILE:HG23  | 6        | 0.88          |
| (1,1583) | 1:45:A:ASN:HD21  | 1:44:A:ILE:HD11  | 5        | 0.88          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21  | 18       | 0.88          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21  | 18       | 0.88          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 2        | 0.88          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB3   | 4        | 0.88          |
| (1,922)  | 1:116:B:ALA:HB1  | 1:115:B:LYS:HA   | 9        | 0.88          |
| (1,840)  | 1:36:B:VAL:HG13  | 1:37:B:MET:HG3   | 5        | 0.88          |
| (1,839)  | 1:36:A:VAL:HG13  | 1:37:A:MET:HG3   | 5        | 0.88          |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2   | 13       | 0.88          |
| (1,547)  | 1:92:A:MET:HE2   | 1:92:A:MET:HB2   | 13       | 0.88          |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 9        | 0.88          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG21  | 1        | 0.88          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG21  | 5        | 0.88          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG21  | 18       | 0.88          |
| (1,428)  | 1:87:B:VAL:HG13  | 1:87:B:VAL:HG23  | 19       | 0.88          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG21  | 1        | 0.88          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG21  | 5        | 0.88          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG21  | 18       | 0.88          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG22  | 17       | 0.88          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG22  | 17       | 0.88          |
| (1,52)   | 1:42:B:VAL:HG21  | 1:42:B:VAL:HG11  | 5        | 0.88          |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG12  | 16       | 0.88          |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG12  | 19       | 0.88          |
| (1,52)   | 1:42:B:VAL:HG23  | 1:42:B:VAL:HG13  | 20       | 0.88          |
| (1,51)   | 1:42:A:VAL:HG23  | 1:42:A:VAL:HG12  | 4        | 0.88          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG12  | 19       | 0.88          |
| (1,51)   | 1:42:A:VAL:HG23  | 1:42:A:VAL:HG13  | 20       | 0.88          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 7        | 0.87          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG22  | 1        | 0.87          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 8        | 0.87          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 8        | 0.87          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG23  | 5        | 0.87          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG23  | 5        | 0.87          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB2   | 16       | 0.87          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB2   | 20       | 0.87          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB2   | 16       | 0.87          |
| (1,921)  | 1:116:A:ALA:HB1  | 1:115:A:LYS:HA   | 9        | 0.87          |
| (1,839)  | 1:36:A:VAL:HG11  | 1:37:A:MET:HG3   | 2        | 0.87          |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2   | 20       | 0.87          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG22  | 4        | 0.87          |
| (1,428)  | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG23  | 12       | 0.87          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG21  | 15       | 0.87          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG22  | 4        | 0.87          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG21  | 15       | 0.87          |
| (1,288)  | 1:106:B:THR:HG23 | 1:85:B:THR:HG23  | 2        | 0.87          |
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG22  | 18       | 0.87          |
| (1,287)  | 1:106:A:THR:HG23 | 1:85:A:THR:HG23  | 2        | 0.87          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG22  | 18       | 0.87          |
| (1,72)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG2   | 10       | 0.87          |
| (1,71)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG2   | 10       | 0.87          |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG13  | 12       | 0.87          |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG12  | 14       | 0.87          |
| (1,51)   | 1:42:A:VAL:HG21  | 1:42:A:VAL:HG13  | 11       | 0.87          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG13  | 12       | 0.87          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG12  | 14       | 0.87          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 13       | 0.86          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG22  | 1        | 0.86          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 18       | 0.86          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 18       | 0.86          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG13 | 19       | 0.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD21 | 1        | 0.86          |
| (1,2074) | 1:88:B:LYS:H     | 1:88:B:LYS:HB2   | 9        | 0.86          |
| (1,2073) | 1:88:A:LYS:H     | 1:88:A:LYS:HB2   | 9        | 0.86          |
| (1,1584) | 1:45:B:ASN:HD21  | 1:44:B:ILE:HD11  | 5        | 0.86          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 12       | 0.86          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 12       | 0.86          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 1        | 0.86          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 13       | 0.86          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 1        | 0.86          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 13       | 0.86          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB2   | 20       | 0.86          |
| (1,908)  | 1:5:B:PRO:HA     | 1:9:B:ARG:HB2    | 8        | 0.86          |
| (1,907)  | 1:5:A:PRO:HA     | 1:9:A:ARG:HB2    | 8        | 0.86          |
| (1,840)  | 1:36:B:VAL:HG11  | 1:37:B:MET:HG3   | 2        | 0.86          |
| (1,840)  | 1:36:B:VAL:HG11  | 1:37:B:MET:HG3   | 14       | 0.86          |
| (1,839)  | 1:36:A:VAL:HG11  | 1:37:A:MET:HG3   | 14       | 0.86          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG12 | 3        | 0.86          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG12 | 3        | 0.86          |
| (1,547)  | 1:92:A:MET:HE2   | 1:92:A:MET:HB2   | 20       | 0.86          |
| (1,543)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD22  | 14       | 0.86          |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 16       | 0.86          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 16       | 0.86          |
| (1,428)  | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG21  | 16       | 0.86          |
| (1,427)  | 1:87:A:VAL:HG13  | 1:87:A:VAL:HG23  | 6        | 0.86          |
| (1,427)  | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG23  | 12       | 0.86          |
| (1,52)   | 1:42:B:VAL:HG21  | 1:42:B:VAL:HG11  | 3        | 0.86          |
| (1,52)   | 1:42:B:VAL:HG21  | 1:42:B:VAL:HG13  | 11       | 0.86          |
| (1,51)   | 1:42:A:VAL:HG21  | 1:42:A:VAL:HG11  | 3        | 0.86          |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG11 | 20       | 0.85          |
| (1,2735) | 1:51:A:GLN:HE21  | 1:90:A:LEU:H     | 19       | 0.85          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG22  | 3        | 0.85          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG22  | 3        | 0.85          |
| (1,2552) | 1:76:B:TRP:HE1   | 1:75:B:HIS:HB2   | 10       | 0.85          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 14       | 0.85          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 16       | 0.85          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 14       | 0.85          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 16       | 0.85          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD21 | 1        | 0.85          |
| (1,1728) | 1:76:B:TRP:H     | 1:73:B:SER:HB3   | 7        | 0.85          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 2        | 0.85          |
| (1,1449) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HE1   | 2        | 0.85          |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB3   | 11       | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB3   | 11       | 0.85          |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG12  | 2        | 0.85          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 6        | 0.85          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 8        | 0.85          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB3   | 18       | 0.85          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 8        | 0.85          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB3   | 18       | 0.85          |
| (1,922)  | 1:116:B:ALA:HB2  | 1:115:B:LYS:HA   | 1        | 0.85          |
| (1,921)  | 1:116:A:ALA:HB2  | 1:115:A:LYS:HA   | 1        | 0.85          |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG12 | 5        | 0.85          |
| (1,761)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG12 | 5        | 0.85          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 7        | 0.85          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 7        | 0.85          |
| (1,548)  | 1:92:B:MET:HE1   | 1:92:B:MET:HB2   | 5        | 0.85          |
| (1,547)  | 1:92:A:MET:HE1   | 1:92:A:MET:HB2   | 5        | 0.85          |
| (1,544)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD22  | 14       | 0.85          |
| (1,428)  | 1:87:B:VAL:HG13  | 1:87:B:VAL:HG23  | 6        | 0.85          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG23  | 9        | 0.85          |
| (1,428)  | 1:87:B:VAL:HG11  | 1:87:B:VAL:HG22  | 11       | 0.85          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG23  | 9        | 0.85          |
| (1,427)  | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG22  | 11       | 0.85          |
| (1,427)  | 1:87:A:VAL:HG11  | 1:87:A:VAL:HG21  | 16       | 0.85          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG13  | 5        | 0.85          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG13  | 5        | 0.85          |
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG23  | 12       | 0.85          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG23  | 12       | 0.85          |
| (1,52)   | 1:42:B:VAL:HG22  | 1:42:B:VAL:HG13  | 15       | 0.85          |
| (1,51)   | 1:42:A:VAL:HG22  | 1:42:A:VAL:HG13  | 15       | 0.85          |
| (1,3090) | 1:112:B:LEU:HD21 | 1:14:A:VAL:HA    | 19       | 0.84          |
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 17       | 0.84          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 17       | 0.84          |
| (1,2736) | 1:51:B:GLN:HE21  | 1:90:B:LEU:H     | 19       | 0.84          |
| (1,2551) | 1:76:A:TRP:HE1   | 1:75:A:HIS:HB2   | 10       | 0.84          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 3        | 0.84          |
| (1,1996) | 1:67:B:GLY:H     | 1:64:B:VAL:HB    | 12       | 0.84          |
| (1,1995) | 1:67:A:GLY:H     | 1:64:A:VAL:HB    | 12       | 0.84          |
| (1,1727) | 1:76:A:TRP:H     | 1:73:A:SER:HB3   | 7        | 0.84          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 16       | 0.84          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 16       | 0.84          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 10       | 0.84          |
| (1,1449) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HE1   | 10       | 0.84          |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB3   | 14       | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB3   | 14       | 0.84          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG11  | 4        | 0.84          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG11  | 4        | 0.84          |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG12  | 2        | 0.84          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 6        | 0.84          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 6        | 0.84          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 6        | 0.84          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 11       | 0.84          |
| (1,922)  | 1:116:B:ALA:HB2  | 1:115:B:LYS:HA   | 18       | 0.84          |
| (1,921)  | 1:116:A:ALA:HB2  | 1:115:A:LYS:HA   | 18       | 0.84          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB1  | 16       | 0.84          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB1  | 16       | 0.84          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB1  | 20       | 0.84          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22  | 11       | 0.84          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22  | 11       | 0.84          |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG13 | 1        | 0.84          |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG12 | 4        | 0.84          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG12 | 6        | 0.84          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG13 | 12       | 0.84          |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG13 | 13       | 0.84          |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG11 | 20       | 0.84          |
| (1,761)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG13 | 1        | 0.84          |
| (1,761)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG12 | 4        | 0.84          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG12 | 6        | 0.84          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG11 | 10       | 0.84          |
| (1,761)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG13 | 13       | 0.84          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG11 | 15       | 0.84          |
| (1,761)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG11 | 20       | 0.84          |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 17       | 0.84          |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 17       | 0.84          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG22  | 7        | 0.84          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG22  | 8        | 0.84          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG22  | 7        | 0.84          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG22  | 8        | 0.84          |
| (1,336)  | 1:36:B:VAL:HG12  | 1:30:B:ASP:HB2   | 16       | 0.84          |
| (1,335)  | 1:36:A:VAL:HG12  | 1:30:A:ASP:HB2   | 16       | 0.84          |
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG23  | 20       | 0.84          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG23  | 20       | 0.84          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 4        | 0.84          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 4        | 0.84          |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 3        | 0.83          |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 3        | 0.83          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 9        | 0.83          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 9        | 0.83          |
| (1,3068) | 1:70:B:GLY:HA2   | 1:71:A:ILE:HG22  | 3        | 0.83          |
| (1,3067) | 1:70:A:GLY:HA2   | 1:71:B:ILE:HG22  | 3        | 0.83          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 3        | 0.83          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 5        | 0.83          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 5        | 0.83          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB2   | 16       | 0.83          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 16       | 0.83          |
| (1,2160) | 1:77:B:ASN:H     | 1:115:B:LYS:HG2  | 1        | 0.83          |
| (1,2155) | 1:77:A:ASN:H     | 1:114:A:ARG:HA   | 7        | 0.83          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG21  | 7        | 0.83          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG21  | 7        | 0.83          |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB3   | 8        | 0.83          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 11       | 0.83          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 17       | 0.83          |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG12 | 17       | 0.83          |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG12 | 17       | 0.83          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB1  | 20       | 0.83          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23  | 5        | 0.83          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23  | 5        | 0.83          |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG11 | 2        | 0.83          |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG11 | 8        | 0.83          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG11 | 9        | 0.83          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG11 | 10       | 0.83          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG11 | 15       | 0.83          |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG12 | 19       | 0.83          |
| (1,761)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG11 | 2        | 0.83          |
| (1,761)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG11 | 8        | 0.83          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG13 | 12       | 0.83          |
| (1,761)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG12 | 19       | 0.83          |
| (1,428)  | 1:87:B:VAL:HG12  | 1:87:B:VAL:HG22  | 10       | 0.83          |
| (1,427)  | 1:87:A:VAL:HG12  | 1:87:A:VAL:HG22  | 10       | 0.83          |
| (1,312)  | 1:71:B:ILE:HG22  | 1:71:B:ILE:HG13  | 1        | 0.83          |
| (1,311)  | 1:71:A:ILE:HG22  | 1:71:A:ILE:HG13  | 1        | 0.83          |
| (1,3101) | 1:9:A:ARG:HB2    | 1:115:B:LYS:HA   | 11       | 0.82          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB3  | 5        | 0.82          |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG12 | 14       | 0.82          |
| (1,2159) | 1:77:A:ASN:H     | 1:115:A:LYS:HG2  | 1        | 0.82          |
| (1,2156) | 1:77:B:ASN:H     | 1:114:B:ARG:HA   | 7        | 0.82          |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB3   | 3        | 0.82          |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB3   | 3        | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB3   | 8        | 0.82          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB1   | 3        | 0.82          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 3        | 0.82          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB1   | 17       | 0.82          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG11 | 14       | 0.82          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG11 | 9        | 0.82          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG11 | 14       | 0.82          |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG11  | 15       | 0.82          |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG13  | 14       | 0.82          |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG11  | 15       | 0.82          |
| (1,355)  | 1:41:A:GLU:HG2   | 1:48:A:VAL:HA    | 17       | 0.82          |
| (1,312)  | 1:71:B:ILE:HG22  | 1:71:B:ILE:HG13  | 4        | 0.82          |
| (1,312)  | 1:71:B:ILE:HG23  | 1:71:B:ILE:HG13  | 5        | 0.82          |
| (1,312)  | 1:71:B:ILE:HG21  | 1:71:B:ILE:HG13  | 7        | 0.82          |
| (1,312)  | 1:71:B:ILE:HG23  | 1:71:B:ILE:HG13  | 19       | 0.82          |
| (1,311)  | 1:71:A:ILE:HG22  | 1:71:A:ILE:HG13  | 4        | 0.82          |
| (1,311)  | 1:71:A:ILE:HG23  | 1:71:A:ILE:HG13  | 5        | 0.82          |
| (1,311)  | 1:71:A:ILE:HG21  | 1:71:A:ILE:HG13  | 7        | 0.82          |
| (1,311)  | 1:71:A:ILE:HG23  | 1:71:A:ILE:HG13  | 8        | 0.82          |
| (1,311)  | 1:71:A:ILE:HG23  | 1:71:A:ILE:HG13  | 19       | 0.82          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 10       | 0.82          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 10       | 0.82          |
| (1,3102) | 1:9:B:ARG:HB2    | 1:115:A:LYS:HA   | 20       | 0.81          |
| (1,3089) | 1:112:A:LEU:HD21 | 1:14:B:VAL:HA    | 19       | 0.81          |
| (1,3082) | 1:12:B:PHE:H     | 1:111:A:VAL:HG22 | 8        | 0.81          |
| (1,3071) | 1:44:A:ILE:HD13  | 1:99:B:TRP:HE1   | 2        | 0.81          |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG11 | 20       | 0.81          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG12 | 14       | 0.81          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB3   | 10       | 0.81          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB3   | 10       | 0.81          |
| (1,1476) | 1:112:B:LEU:HD13 | 1:71:B:ILE:HA    | 7        | 0.81          |
| (1,1475) | 1:112:A:LEU:HD13 | 1:71:A:ILE:HA    | 7        | 0.81          |
| (1,1388) | 1:20:B:VAL:HG13  | 1:19:B:SER:H     | 3        | 0.81          |
| (1,1387) | 1:20:A:VAL:HG13  | 1:19:A:SER:H     | 3        | 0.81          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21  | 4        | 0.81          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21  | 4        | 0.81          |
| (1,936)  | 1:98:B:ALA:HA    | 1:97:B:ALA:HB3   | 12       | 0.81          |
| (1,935)  | 1:98:A:ALA:HA    | 1:97:A:ALA:HB3   | 12       | 0.81          |
| (1,762)  | 1:109:B:VAL:HG23 | 1:109:B:VAL:HG12 | 16       | 0.81          |
| (1,761)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HG12 | 16       | 0.81          |
| (1,542)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD11  | 4        | 0.81          |
| (1,541)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD11  | 4        | 0.81          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 10       | 0.81          |
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 10       | 0.81          |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG13  | 14       | 0.81          |
| (1,356)  | 1:41:B:GLU:HG2   | 1:48:B:VAL:HA    | 17       | 0.81          |
| (1,312)  | 1:71:B:ILE:HG21  | 1:71:B:ILE:HG13  | 6        | 0.81          |
| (1,312)  | 1:71:B:ILE:HG23  | 1:71:B:ILE:HG13  | 8        | 0.81          |
| (1,311)  | 1:71:A:ILE:HG21  | 1:71:A:ILE:HG13  | 6        | 0.81          |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD12  | 10       | 0.8           |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD12  | 10       | 0.8           |
| (1,3102) | 1:9:B:ARG:HB2    | 1:115:A:LYS:HA   | 11       | 0.8           |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB3  | 5        | 0.8           |
| (1,3067) | 1:70:A:GLY:HA3   | 1:71:B:ILE:HG22  | 13       | 0.8           |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 4        | 0.8           |
| (1,2074) | 1:88:B:LYS:H     | 1:88:B:LYS:HB2   | 20       | 0.8           |
| (1,2073) | 1:88:A:LYS:H     | 1:88:A:LYS:HB2   | 20       | 0.8           |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 1        | 0.8           |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 1        | 0.8           |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 15       | 0.8           |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 15       | 0.8           |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB2   | 16       | 0.8           |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB3   | 20       | 0.8           |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB2   | 16       | 0.8           |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB3   | 20       | 0.8           |
| (1,1216) | 1:22:B:VAL:HG11  | 1:20:B:VAL:HB    | 4        | 0.8           |
| (1,1215) | 1:22:A:VAL:HG11  | 1:20:A:VAL:HB    | 4        | 0.8           |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 18       | 0.8           |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 18       | 0.8           |
| (1,1020) | 1:12:B:PHE:HB3   | 1:13:B:SER:HB2   | 15       | 0.8           |
| (1,1019) | 1:12:A:PHE:HB3   | 1:13:A:SER:HB2   | 15       | 0.8           |
| (1,924)  | 1:81:B:THR:HG22  | 1:111:B:VAL:HG11 | 19       | 0.8           |
| (1,923)  | 1:81:A:THR:HG22  | 1:111:A:VAL:HG11 | 19       | 0.8           |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23  | 20       | 0.8           |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23  | 20       | 0.8           |
| (1,762)  | 1:109:B:VAL:HG22 | 1:109:B:VAL:HG13 | 17       | 0.8           |
| (1,761)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HG13 | 17       | 0.8           |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 11       | 0.8           |
| (1,462)  | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 18       | 0.8           |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 11       | 0.8           |
| (1,461)  | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 18       | 0.8           |
| (1,312)  | 1:71:B:ILE:HG22  | 1:71:B:ILE:HG13  | 2        | 0.8           |
| (1,312)  | 1:71:B:ILE:HG21  | 1:71:B:ILE:HG13  | 11       | 0.8           |
| (1,312)  | 1:71:B:ILE:HG22  | 1:71:B:ILE:HG13  | 12       | 0.8           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,311)  | 1:71:A:ILE:HG22  | 1:71:A:ILE:HG13  | 2        | 0.8           |
| (1,311)  | 1:71:A:ILE:HG21  | 1:71:A:ILE:HG13  | 11       | 0.8           |
| (1,311)  | 1:71:A:ILE:HG22  | 1:71:A:ILE:HG13  | 12       | 0.8           |
| (1,288)  | 1:106:B:THR:HG23 | 1:85:B:THR:HG21  | 13       | 0.8           |
| (1,288)  | 1:106:B:THR:HG21 | 1:85:B:THR:HG22  | 19       | 0.8           |
| (1,287)  | 1:106:A:THR:HG23 | 1:85:A:THR:HG21  | 13       | 0.8           |
| (1,287)  | 1:106:A:THR:HG21 | 1:85:A:THR:HG22  | 19       | 0.8           |
| (1,3099) | 1:9:A:ARG:HB2    | 1:117:B:VAL:HG21 | 18       | 0.79          |
| (1,3081) | 1:12:A:PHE:H     | 1:111:B:VAL:HG22 | 8        | 0.79          |
| (1,3076) | 1:42:B:VAL:HG21  | 1:99:A:TRP:HE1   | 20       | 0.79          |
| (1,3068) | 1:70:B:GLY:HA3   | 1:71:A:ILE:HG22  | 13       | 0.79          |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG11 | 7        | 0.79          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 11       | 0.79          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 11       | 0.79          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 4        | 0.79          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG22 | 1        | 0.79          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 12       | 0.79          |
| (1,2083) | 1:88:A:LYS:H     | 1:88:A:LYS:HD2   | 12       | 0.79          |
| (1,1544) | 1:55:B:GLU:HG3   | 1:20:B:VAL:HG22  | 5        | 0.79          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 4        | 0.79          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 2        | 0.79          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 2        | 0.79          |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB3   | 19       | 0.79          |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB3   | 19       | 0.79          |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB3   | 17       | 0.79          |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB3   | 17       | 0.79          |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG13 | 2        | 0.79          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG21  | 1        | 0.79          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG21  | 1        | 0.79          |
| (1,761)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG13 | 11       | 0.79          |
| (1,402)  | 1:102:B:ILE:HD12 | 1:25:B:LYS:HG2   | 2        | 0.79          |
| (1,401)  | 1:102:A:ILE:HD12 | 1:25:A:LYS:HG2   | 2        | 0.79          |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG12  | 8        | 0.79          |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG12  | 8        | 0.79          |
| (1,312)  | 1:71:B:ILE:HG23  | 1:71:B:ILE:HG13  | 10       | 0.79          |
| (1,312)  | 1:71:B:ILE:HG23  | 1:71:B:ILE:HG13  | 16       | 0.79          |
| (1,311)  | 1:71:A:ILE:HG23  | 1:71:A:ILE:HG13  | 10       | 0.79          |
| (1,311)  | 1:71:A:ILE:HG23  | 1:71:A:ILE:HG13  | 16       | 0.79          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 3        | 0.79          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 11       | 0.79          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 3        | 0.79          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 11       | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,288)  | 1:106:B:THR:HG21 | 1:85:B:THR:HG21  | 14       | 0.79          |
| (1,287)  | 1:106:A:THR:HG21 | 1:85:A:THR:HG21  | 14       | 0.79          |
| (1,3101) | 1:9:A:ARG:HB2    | 1:115:B:LYS:HA   | 20       | 0.78          |
| (1,3072) | 1:44:B:ILE:HD13  | 1:99:A:TRP:HE1   | 2        | 0.78          |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG11 | 7        | 0.78          |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG11 | 16       | 0.78          |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG11 | 16       | 0.78          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG23 | 12       | 0.78          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG22 | 1        | 0.78          |
| (1,2084) | 1:88:B:LYS:H     | 1:88:B:LYS:HD2   | 12       | 0.78          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG21  | 15       | 0.78          |
| (1,1543) | 1:55:A:GLU:HG3   | 1:20:A:VAL:HG22  | 5        | 0.78          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 4        | 0.78          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 13       | 0.78          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 7        | 0.78          |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG13 | 2        | 0.78          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG13 | 11       | 0.78          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG13 | 11       | 0.78          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB1  | 14       | 0.78          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB1  | 14       | 0.78          |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG13 | 11       | 0.78          |
| (1,542)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD13  | 11       | 0.78          |
| (1,541)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD13  | 11       | 0.78          |
| (1,312)  | 1:71:B:ILE:HG21  | 1:71:B:ILE:HG13  | 3        | 0.78          |
| (1,311)  | 1:71:A:ILE:HG21  | 1:71:A:ILE:HG13  | 3        | 0.78          |
| (1,311)  | 1:71:A:ILE:HG22  | 1:71:A:ILE:HG13  | 15       | 0.78          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 2        | 0.78          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 2        | 0.78          |
| (1,3100) | 1:9:B:ARG:HB2    | 1:117:A:VAL:HG21 | 18       | 0.77          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 11       | 0.77          |
| (1,3056) | 1:107:B:ALA:HB3  | 1:109:A:VAL:HG13 | 1        | 0.77          |
| (1,3056) | 1:107:B:ALA:HB2  | 1:109:A:VAL:HG12 | 4        | 0.77          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 17       | 0.77          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 17       | 0.77          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD23 | 12       | 0.77          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 12       | 0.77          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 13       | 0.77          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 15       | 0.77          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG21  | 15       | 0.77          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 13       | 0.77          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 7        | 0.77          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG12 | 9        | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG12 | 9        | 0.77          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 15       | 0.77          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 15       | 0.77          |
| (1,312)  | 1:71:B:ILE:HG22  | 1:71:B:ILE:HG13  | 15       | 0.77          |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD12  | 9        | 0.76          |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD12  | 9        | 0.76          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 11       | 0.76          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 7        | 0.76          |
| (1,3075) | 1:42:A:VAL:HG21  | 1:99:B:TRP:HE1   | 20       | 0.76          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 19       | 0.76          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG11  | 13       | 0.76          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG11  | 13       | 0.76          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 6        | 0.76          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 6        | 0.76          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 6        | 0.76          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 13       | 0.76          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 12       | 0.76          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 15       | 0.76          |
| (1,1544) | 1:55:B:GLU:HG3   | 1:20:B:VAL:HG21  | 10       | 0.76          |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG11 | 8        | 0.76          |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG11 | 8        | 0.76          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23  | 15       | 0.76          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23  | 15       | 0.76          |
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG21  | 10       | 0.76          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG21  | 10       | 0.76          |
| (1,180)  | 1:109:B:VAL:HG22 | 1:81:B:THR:HA    | 14       | 0.76          |
| (1,179)  | 1:109:A:VAL:HG22 | 1:81:A:THR:HA    | 14       | 0.76          |
| (1,3068) | 1:70:B:GLY:HA3   | 1:71:A:ILE:HG21  | 10       | 0.75          |
| (1,3067) | 1:70:A:GLY:HA3   | 1:71:B:ILE:HG21  | 10       | 0.75          |
| (1,3055) | 1:107:A:ALA:HB2  | 1:109:B:VAL:HG12 | 4        | 0.75          |
| (1,2735) | 1:51:A:GLN:HE21  | 1:90:A:LEU:H     | 1        | 0.75          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG23  | 8        | 0.75          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 6        | 0.75          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 19       | 0.75          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 12       | 0.75          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 19       | 0.75          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB1   | 18       | 0.75          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB1   | 18       | 0.75          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 20       | 0.75          |
| (1,2151) | 1:77:A:ASN:H     | 1:115:A:LYS:HD2  | 6        | 0.75          |
| (1,2084) | 1:88:B:LYS:H     | 1:88:B:LYS:HD2   | 16       | 0.75          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 18       | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1543) | 1:55:A:GLU:HG3   | 1:20:A:VAL:HG21  | 10       | 0.75          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 4        | 0.75          |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB2   | 7        | 0.75          |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB2   | 7        | 0.75          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG22  | 11       | 0.75          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG22  | 11       | 0.75          |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG21  | 12       | 0.75          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG13 | 12       | 0.75          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG13 | 12       | 0.75          |
| (1,908)  | 1:5:B:PRO:HA     | 1:9:B:ARG:HB2    | 18       | 0.75          |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG11 | 7        | 0.75          |
| (1,762)  | 1:109:B:VAL:HG21 | 1:109:B:VAL:HG12 | 18       | 0.75          |
| (1,761)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG11 | 7        | 0.75          |
| (1,761)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HG12 | 18       | 0.75          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 2        | 0.75          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 2        | 0.75          |
| (1,3055) | 1:107:A:ALA:HB3  | 1:109:B:VAL:HG13 | 1        | 0.74          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 17       | 0.74          |
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 20       | 0.74          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 20       | 0.74          |
| (1,2736) | 1:51:B:GLN:HE21  | 1:90:B:LEU:H     | 1        | 0.74          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG23  | 8        | 0.74          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 11       | 0.74          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 20       | 0.74          |
| (1,2152) | 1:77:B:ASN:H     | 1:115:B:LYS:HD2  | 6        | 0.74          |
| (1,2083) | 1:88:A:LYS:H     | 1:88:A:LYS:HD2   | 16       | 0.74          |
| (1,1909) | 1:72:A:ASP:H     | 1:71:A:ILE:HG21  | 4        | 0.74          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 18       | 0.74          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 4        | 0.74          |
| (1,1481) | 1:112:A:LEU:HD13 | 1:76:A:TRP:HB2   | 14       | 0.74          |
| (1,1430) | 1:102:B:ILE:HD11 | 1:28:B:ALA:HB1   | 12       | 0.74          |
| (1,1429) | 1:102:A:ILE:HD11 | 1:28:A:ALA:HB1   | 12       | 0.74          |
| (1,1216) | 1:22:B:VAL:HG13  | 1:20:B:VAL:HB    | 6        | 0.74          |
| (1,1215) | 1:22:A:VAL:HG13  | 1:20:A:VAL:HB    | 6        | 0.74          |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG21  | 12       | 0.74          |
| (1,922)  | 1:116:B:ALA:HB2  | 1:115:B:LYS:HA   | 10       | 0.74          |
| (1,921)  | 1:116:A:ALA:HB2  | 1:115:A:LYS:HA   | 10       | 0.74          |
| (1,907)  | 1:5:A:PRO:HA     | 1:9:A:ARG:HB2    | 18       | 0.74          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG21  | 13       | 0.74          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG21  | 13       | 0.74          |
| (1,48)   | 1:42:B:VAL:HG21  | 1:44:B:ILE:HB    | 7        | 0.74          |
| (1,47)   | 1:42:A:VAL:HG21  | 1:44:A:ILE:HB    | 7        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 7        | 0.73          |
| (1,3085) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HG23  | 12       | 0.73          |
| (1,3052) | 1:21:B:TRP:HE1   | 1:31:A:ILE:HD13  | 9        | 0.73          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 17       | 0.73          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 9        | 0.73          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 11       | 0.73          |
| (1,2218) | 1:118:B:ARG:H    | 1:118:B:ARG:HG3  | 14       | 0.73          |
| (1,2217) | 1:118:A:ARG:H    | 1:118:A:ARG:HG3  | 14       | 0.73          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 9        | 0.73          |
| (1,2160) | 1:77:B:ASN:H     | 1:115:B:LYS:HG2  | 17       | 0.73          |
| (1,2151) | 1:77:A:ASN:H     | 1:115:A:LYS:HD2  | 8        | 0.73          |
| (1,1910) | 1:72:B:ASP:H     | 1:71:B:ILE:HG21  | 4        | 0.73          |
| (1,1844) | 1:96:B:GLN:HE22  | 1:95:B:LYS:HA    | 20       | 0.73          |
| (1,1843) | 1:96:A:GLN:HE22  | 1:95:A:LYS:HA    | 20       | 0.73          |
| (1,1482) | 1:112:B:LEU:HD13 | 1:76:B:TRP:HB2   | 14       | 0.73          |
| (1,1430) | 1:102:B:ILE:HD11 | 1:28:B:ALA:HB3   | 10       | 0.73          |
| (1,1387) | 1:20:A:VAL:HG12  | 1:19:A:SER:H     | 18       | 0.73          |
| (1,840)  | 1:36:B:VAL:HG13  | 1:37:B:MET:HG3   | 4        | 0.73          |
| (1,839)  | 1:36:A:VAL:HG13  | 1:37:A:MET:HG3   | 4        | 0.73          |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG21  | 12       | 0.73          |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG23  | 18       | 0.73          |
| (1,660)  | 1:51:B:GLN:H     | 1:42:B:VAL:HG11  | 11       | 0.73          |
| (1,659)  | 1:51:A:GLN:H     | 1:42:A:VAL:HG11  | 11       | 0.73          |
| (1,596)  | 1:107:B:ALA:HB2  | 1:106:B:THR:HA   | 15       | 0.73          |
| (1,595)  | 1:107:A:ALA:HB2  | 1:106:A:THR:HA   | 15       | 0.73          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG11  | 6        | 0.73          |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG11  | 18       | 0.73          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG11  | 6        | 0.73          |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG11  | 18       | 0.73          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD23 | 13       | 0.72          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB2  | 11       | 0.72          |
| (1,3067) | 1:70:A:GLY:HA3   | 1:71:B:ILE:HG23  | 7        | 0.72          |
| (1,3051) | 1:21:A:TRP:HE1   | 1:31:B:ILE:HD13  | 9        | 0.72          |
| (1,2997) | 1:77:A:ASN:HD22  | 1:115:A:LYS:H    | 19       | 0.72          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 8        | 0.72          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 8        | 0.72          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 9        | 0.72          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB2   | 1        | 0.72          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 1        | 0.72          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 7        | 0.72          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 9        | 0.72          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 7        | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2159) | 1:77:A:ASN:H     | 1:115:A:LYS:HG2  | 17       | 0.72          |
| (1,2152) | 1:77:B:ASN:H     | 1:115:B:LYS:HD2  | 8        | 0.72          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 8        | 0.72          |
| (1,1544) | 1:55:B:GLU:HG3   | 1:20:B:VAL:HG22  | 11       | 0.72          |
| (1,1543) | 1:55:A:GLU:HG3   | 1:20:A:VAL:HG22  | 11       | 0.72          |
| (1,1429) | 1:102:A:ILE:HD11 | 1:28:A:ALA:HB3   | 10       | 0.72          |
| (1,1388) | 1:20:B:VAL:HG12  | 1:19:B:SER:H     | 18       | 0.72          |
| (1,1314) | 1:70:B:GLY:H     | 1:64:B:VAL:HG11  | 9        | 0.72          |
| (1,1313) | 1:70:A:GLY:H     | 1:64:A:VAL:HG11  | 9        | 0.72          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 3        | 0.72          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 3        | 0.72          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 4        | 0.72          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 4        | 0.72          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 14       | 0.72          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 14       | 0.72          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG23  | 16       | 0.72          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG23  | 16       | 0.72          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 3        | 0.72          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 3        | 0.72          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG11 | 14       | 0.72          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG11 | 14       | 0.72          |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG21  | 12       | 0.72          |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG23  | 18       | 0.72          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22  | 9        | 0.72          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22  | 9        | 0.72          |
| (1,662)  | 1:42:B:VAL:HG11  | 1:90:B:LEU:HG    | 18       | 0.72          |
| (1,661)  | 1:42:A:VAL:HG11  | 1:90:A:LEU:HG    | 18       | 0.72          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 4        | 0.72          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 20       | 0.72          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 20       | 0.72          |
| (1,543)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD23  | 18       | 0.72          |
| (1,542)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD11  | 5        | 0.72          |
| (1,288)  | 1:106:B:THR:HG21 | 1:85:B:THR:HG21  | 3        | 0.72          |
| (1,287)  | 1:106:A:THR:HG21 | 1:85:A:THR:HG21  | 3        | 0.72          |
| (1,54)   | 1:42:B:VAL:HG23  | 1:99:B:TRP:HZ2   | 20       | 0.72          |
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB    | 19       | 0.72          |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB    | 19       | 0.72          |
| (1,3086) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HG23  | 12       | 0.71          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 2        | 0.71          |
| (1,2998) | 1:77:B:ASN:HD22  | 1:115:B:LYS:H    | 19       | 0.71          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 2        | 0.71          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 2        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 10       | 0.71          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 10       | 0.71          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 8        | 0.71          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 6        | 0.71          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 6        | 0.71          |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB3   | 6        | 0.71          |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB3   | 6        | 0.71          |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB3   | 19       | 0.71          |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB3   | 19       | 0.71          |
| (1,1215) | 1:22:A:VAL:HG12  | 1:20:A:VAL:HB    | 18       | 0.71          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG22  | 14       | 0.71          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG22  | 14       | 0.71          |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG22  | 2        | 0.71          |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG21  | 14       | 0.71          |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG22  | 16       | 0.71          |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG22  | 19       | 0.71          |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG22  | 2        | 0.71          |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG21  | 14       | 0.71          |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG22  | 16       | 0.71          |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG22  | 19       | 0.71          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22  | 3        | 0.71          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22  | 3        | 0.71          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 4        | 0.71          |
| (1,544)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD23  | 18       | 0.71          |
| (1,541)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD11  | 5        | 0.71          |
| (1,426)  | 1:87:B:VAL:HG13  | 1:53:B:PHE:HE1   | 19       | 0.71          |
| (1,425)  | 1:87:A:VAL:HG13  | 1:53:A:PHE:HE1   | 19       | 0.71          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG23  | 8        | 0.71          |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG23  | 8        | 0.71          |
| (1,180)  | 1:109:B:VAL:HG23 | 1:81:B:THR:HA    | 11       | 0.71          |
| (1,53)   | 1:42:A:VAL:HG23  | 1:99:A:TRP:HZ2   | 20       | 0.71          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD23 | 13       | 0.7           |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 2        | 0.7           |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB2  | 11       | 0.7           |
| (1,3068) | 1:70:B:GLY:HA3   | 1:71:A:ILE:HG23  | 7        | 0.7           |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG23 | 16       | 0.7           |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 16       | 0.7           |
| (1,2254) | 1:77:B:ASN:HD22  | 1:114:B:ARG:HA   | 19       | 0.7           |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 12       | 0.7           |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 12       | 0.7           |
| (1,1606) | 1:24:B:ASP:H     | 1:25:B:LYS:H     | 4        | 0.7           |
| (1,1605) | 1:24:A:ASP:H     | 1:25:A:LYS:H     | 4        | 0.7           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1544) | 1:55:B:GLU:HG3   | 1:20:B:VAL:HG22 | 3        | 0.7           |
| (1,1543) | 1:55:A:GLU:HG3   | 1:20:A:VAL:HG22 | 3        | 0.7           |
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H    | 20       | 0.7           |
| (1,1216) | 1:22:B:VAL:HG12  | 1:20:B:VAL:HB   | 18       | 0.7           |
| (1,926)  | 1:111:B:VAL:HG11 | 1:79:B:TYR:HE1  | 6        | 0.7           |
| (1,925)  | 1:111:A:VAL:HG11 | 1:79:A:TYR:HE1  | 6        | 0.7           |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG23 | 6        | 0.7           |
| (1,772)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HG22 | 11       | 0.7           |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG23 | 15       | 0.7           |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG23 | 6        | 0.7           |
| (1,771)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HG22 | 11       | 0.7           |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG23 | 15       | 0.7           |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23 | 4        | 0.7           |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1  | 6        | 0.7           |
| (1,667)  | 1:42:A:VAL:HG11  | 1:99:A:TRP:HZ2  | 9        | 0.7           |
| (1,662)  | 1:42:B:VAL:HG11  | 1:90:B:LEU:HG   | 4        | 0.7           |
| (1,661)  | 1:42:A:VAL:HG11  | 1:90:A:LEU:HG   | 4        | 0.7           |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2 | 10       | 0.7           |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2 | 10       | 0.7           |
| (1,400)  | 1:102:B:ILE:HD12 | 1:87:B:VAL:HG23 | 10       | 0.7           |
| (1,179)  | 1:109:A:VAL:HG23 | 1:81:A:THR:HA   | 11       | 0.7           |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3 | 20       | 0.69          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3 | 20       | 0.69          |
| (1,2253) | 1:77:A:ASN:HD22  | 1:114:A:ARG:HA  | 19       | 0.69          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB3  | 9        | 0.69          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB3  | 9        | 0.69          |
| (1,1881) | 1:21:A:TRP:H     | 1:21:A:TRP:HZ2  | 11       | 0.69          |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB3  | 1        | 0.69          |
| (1,1388) | 1:20:B:VAL:HG11  | 1:19:B:SER:H    | 20       | 0.69          |
| (1,1314) | 1:70:B:GLY:H     | 1:64:B:VAL:HG13 | 13       | 0.69          |
| (1,1313) | 1:70:A:GLY:H     | 1:64:A:VAL:HG13 | 13       | 0.69          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21 | 11       | 0.69          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21 | 11       | 0.69          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB   | 16       | 0.69          |
| (1,772)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HG22 | 7        | 0.69          |
| (1,772)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HG22 | 9        | 0.69          |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG21 | 13       | 0.69          |
| (1,771)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HG22 | 7        | 0.69          |
| (1,771)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HG22 | 9        | 0.69          |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG21 | 13       | 0.69          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23 | 4        | 0.69          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1  | 6        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,668)  | 1:42:B:VAL:HG11  | 1:99:B:TRP:HZ2   | 9        | 0.69          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 3        | 0.69          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 3        | 0.69          |
| (1,542)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD12  | 13       | 0.69          |
| (1,542)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD12  | 19       | 0.69          |
| (1,541)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD12  | 13       | 0.69          |
| (1,541)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD12  | 19       | 0.69          |
| (1,399)  | 1:102:A:ILE:HD12 | 1:87:A:VAL:HG23  | 10       | 0.69          |
| (1,344)  | 1:48:B:VAL:HG13  | 1:41:B:GLU:HG2   | 8        | 0.69          |
| (1,3086) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HG23  | 5        | 0.68          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 19       | 0.68          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 2        | 0.68          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 2        | 0.68          |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG23  | 4        | 0.68          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG23  | 4        | 0.68          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 8        | 0.68          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 8        | 0.68          |
| (1,1492) | 1:71:B:ILE:HD13  | 1:14:B:VAL:HG23  | 9        | 0.68          |
| (1,1491) | 1:71:A:ILE:HD13  | 1:14:A:VAL:HG23  | 9        | 0.68          |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB3   | 1        | 0.68          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 20       | 0.68          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 20       | 0.68          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 16       | 0.68          |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG13 | 18       | 0.68          |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG23  | 4        | 0.68          |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG23  | 4        | 0.68          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22  | 16       | 0.68          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23  | 8        | 0.68          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22  | 16       | 0.68          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 5        | 0.68          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 9        | 0.68          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 5        | 0.68          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 9        | 0.68          |
| (1,343)  | 1:48:A:VAL:HG13  | 1:41:A:GLU:HG2   | 8        | 0.68          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 10       | 0.68          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 10       | 0.68          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG13 | 2        | 0.68          |
| (3,6)    | 1:105:B:ASP:H    | 1:25:B:LYS:HG2   | 5        | 0.67          |
| (3,5)    | 1:105:A:ASP:H    | 1:25:A:LYS:HG2   | 5        | 0.67          |
| (1,3100) | 1:9:B:ARG:HB3    | 1:117:A:VAL:HG22 | 3        | 0.67          |
| (1,3085) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HG23  | 5        | 0.67          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD12  | 18       | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 18       | 0.67          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 18       | 0.67          |
| (1,2608) | 1:107:B:ALA:H    | 1:56:B:THR:HG22  | 5        | 0.67          |
| (1,2607) | 1:107:A:ALA:H    | 1:56:A:THR:HG22  | 5        | 0.67          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 19       | 0.67          |
| (1,1882) | 1:21:B:TRP:H     | 1:21:B:TRP:HZ2   | 11       | 0.67          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 17       | 0.67          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 17       | 0.67          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG21  | 8        | 0.67          |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB2   | 4        | 0.67          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 10       | 0.67          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 10       | 0.67          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 10       | 0.67          |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG13 | 18       | 0.67          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB3  | 6        | 0.67          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB3  | 6        | 0.67          |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG21  | 5        | 0.67          |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG23  | 10       | 0.67          |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG21  | 5        | 0.67          |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG23  | 10       | 0.67          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23  | 8        | 0.67          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22  | 6        | 0.67          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG13 | 2        | 0.67          |
| (1,10)   | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG11 | 3        | 0.67          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG13 | 5        | 0.67          |
| (1,10)   | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG12 | 6        | 0.67          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG13 | 5        | 0.67          |
| (1,9)    | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG12 | 6        | 0.67          |
| (1,3099) | 1:9:A:ARG:HB3    | 1:117:B:VAL:HG22 | 3        | 0.66          |
| (1,3076) | 1:42:B:VAL:HG22  | 1:99:A:TRP:HE1   | 17       | 0.66          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG13 | 2        | 0.66          |
| (1,3055) | 1:107:A:ALA:HB2  | 1:109:B:VAL:HG11 | 8        | 0.66          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 1        | 0.66          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 5        | 0.66          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 1        | 0.66          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 5        | 0.66          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG23 | 14       | 0.66          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB1   | 5        | 0.66          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB1   | 5        | 0.66          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 19       | 0.66          |
| (1,1926) | 1:72:B:ASP:H     | 1:71:B:ILE:HD13  | 6        | 0.66          |
| (1,1925) | 1:72:A:ASP:H     | 1:71:A:ILE:HD13  | 6        | 0.66          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2  | 11       | 0.66          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG21 | 8        | 0.66          |
| (1,1430) | 1:102:B:ILE:HD13 | 1:28:B:ALA:HB1  | 13       | 0.66          |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB2  | 4        | 0.66          |
| (1,1429) | 1:102:A:ILE:HD13 | 1:28:A:ALA:HB1  | 13       | 0.66          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21 | 10       | 0.66          |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG21 | 1        | 0.66          |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG21 | 1        | 0.66          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22 | 6        | 0.66          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22 | 7        | 0.66          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22 | 7        | 0.66          |
| (1,662)  | 1:42:B:VAL:HG11  | 1:90:B:LEU:HG   | 3        | 0.66          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG   | 8        | 0.66          |
| (1,662)  | 1:42:B:VAL:HG12  | 1:90:B:LEU:HG   | 14       | 0.66          |
| (1,661)  | 1:42:A:VAL:HG11  | 1:90:A:LEU:HG   | 3        | 0.66          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG   | 8        | 0.66          |
| (1,661)  | 1:42:A:VAL:HG12  | 1:90:A:LEU:HG   | 14       | 0.66          |
| (1,288)  | 1:106:B:THR:HG21 | 1:85:B:THR:HG22 | 6        | 0.66          |
| (1,287)  | 1:106:A:THR:HG21 | 1:85:A:THR:HG22 | 6        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 1        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 2        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 3        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 5        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 6        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 7        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 8        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 9        | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 11       | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 13       | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 14       | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 15       | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 16       | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 17       | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 18       | 0.66          |
| (1,66)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HD2  | 20       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2  | 1        | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2  | 2        | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2  | 3        | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2  | 5        | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2  | 6        | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2  | 7        | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2  | 8        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 9        | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 11       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 13       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 14       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 15       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 16       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 17       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 18       | 0.66          |
| (1,65)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HD2   | 20       | 0.66          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG12 | 10       | 0.66          |
| (1,9)    | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG11 | 3        | 0.66          |
| (1,3080) | 1:11:B:GLU:HG2   | 1:111:A:VAL:HG21 | 10       | 0.65          |
| (1,3076) | 1:42:B:VAL:HG23  | 1:99:A:TRP:HE1   | 2        | 0.65          |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG13 | 2        | 0.65          |
| (1,2555) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HB2  | 2        | 0.65          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 14       | 0.65          |
| (1,2313) | 1:96:A:GLN:HE21  | 1:95:A:LYS:HA    | 7        | 0.65          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG11 | 9        | 0.65          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG12 | 16       | 0.65          |
| (1,2195) | 1:55:A:GLU:H     | 1:22:A:VAL:HG11  | 7        | 0.65          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB1   | 12       | 0.65          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB1   | 12       | 0.65          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 18       | 0.65          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 18       | 0.65          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 11       | 0.65          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG22  | 9        | 0.65          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG22  | 9        | 0.65          |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB1   | 15       | 0.65          |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB3   | 20       | 0.65          |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB1   | 15       | 0.65          |
| (1,1430) | 1:102:B:ILE:HD11 | 1:28:B:ALA:HB3   | 2        | 0.65          |
| (1,1429) | 1:102:A:ILE:HD11 | 1:28:A:ALA:HB3   | 2        | 0.65          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG22  | 19       | 0.65          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG13 | 1        | 0.65          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG13 | 1        | 0.65          |
| (1,772)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HG23  | 8        | 0.65          |
| (1,771)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HG23  | 8        | 0.65          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG21  | 12       | 0.65          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22  | 19       | 0.65          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG21  | 12       | 0.65          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22  | 19       | 0.65          |
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 7        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 7        | 0.65          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG23  | 6        | 0.65          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG23  | 6        | 0.65          |
| (1,390)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG11  | 2        | 0.65          |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG11  | 3        | 0.65          |
| (1,389)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG11  | 2        | 0.65          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG11 | 14       | 0.65          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG12 | 10       | 0.65          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG11 | 14       | 0.65          |
| (1,3094) | 1:86:B:PHE:H     | 1:54:A:PHE:HE2   | 8        | 0.64          |
| (1,3075) | 1:42:A:VAL:HG22  | 1:99:B:TRP:HE1   | 17       | 0.64          |
| (1,3056) | 1:107:B:ALA:HB2  | 1:109:A:VAL:HG11 | 8        | 0.64          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 8        | 0.64          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG13  | 2        | 0.64          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG13  | 2        | 0.64          |
| (1,2556) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HB2  | 2        | 0.64          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG23 | 5        | 0.64          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG11 | 9        | 0.64          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG12 | 16       | 0.64          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 16       | 0.64          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 16       | 0.64          |
| (1,2196) | 1:55:B:GLU:H     | 1:22:B:VAL:HG11  | 7        | 0.64          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 11       | 0.64          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 10       | 0.64          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 11       | 0.64          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 5        | 0.64          |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB3   | 20       | 0.64          |
| (1,1206) | 1:27:B:THR:HA    | 1:26:B:THR:HG21  | 12       | 0.64          |
| (1,1205) | 1:27:A:THR:HA    | 1:26:A:THR:HG21  | 12       | 0.64          |
| (1,1168) | 1:92:B:MET:HE3   | 1:92:B:MET:HG2   | 15       | 0.64          |
| (1,1167) | 1:92:A:MET:HE3   | 1:92:A:MET:HG2   | 15       | 0.64          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG22  | 19       | 0.64          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG13 | 5        | 0.64          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG13 | 5        | 0.64          |
| (1,922)  | 1:116:B:ALA:HB3  | 1:115:B:LYS:HA   | 11       | 0.64          |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG21  | 17       | 0.64          |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG22  | 3        | 0.64          |
| (1,771)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HG21  | 17       | 0.64          |
| (1,771)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HG23  | 20       | 0.64          |
| (1,542)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD13  | 16       | 0.64          |
| (1,541)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD13  | 16       | 0.64          |
| (1,400)  | 1:102:B:ILE:HD12 | 1:87:B:VAL:HG21  | 9        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,399)  | 1:102:A:ILE:HD12 | 1:87:A:VAL:HG21  | 9        | 0.64          |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG11  | 3        | 0.64          |
| (1,252)  | 1:112:B:LEU:HD21 | 1:71:B:ILE:HA    | 14       | 0.64          |
| (1,251)  | 1:112:A:LEU:HD21 | 1:71:A:ILE:HA    | 14       | 0.64          |
| (1,10)   | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG13 | 11       | 0.64          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG11 | 12       | 0.64          |
| (1,9)    | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG13 | 11       | 0.64          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG11 | 12       | 0.64          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 6        | 0.63          |
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG21 | 10       | 0.63          |
| (1,3075) | 1:42:A:VAL:HG23  | 1:99:B:TRP:HE1   | 2        | 0.63          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 8        | 0.63          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 8        | 0.63          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 7        | 0.63          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 7        | 0.63          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 5        | 0.63          |
| (1,2314) | 1:96:B:GLN:HE21  | 1:95:B:LYS:HA    | 7        | 0.63          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB2   | 11       | 0.63          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 11       | 0.63          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 10       | 0.63          |
| (1,1897) | 1:48:A:VAL:H     | 1:48:A:VAL:HG13  | 7        | 0.63          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 5        | 0.63          |
| (1,1436) | 1:38:B:VAL:HG21  | 1:28:B:ALA:HB1   | 12       | 0.63          |
| (1,1435) | 1:38:A:VAL:HG21  | 1:28:A:ALA:HB1   | 12       | 0.63          |
| (1,1430) | 1:102:B:ILE:HD11 | 1:28:B:ALA:HB1   | 9        | 0.63          |
| (1,1429) | 1:102:A:ILE:HD11 | 1:28:A:ALA:HB1   | 9        | 0.63          |
| (1,1403) | 1:20:A:VAL:HG22  | 1:55:A:GLU:HG2   | 9        | 0.63          |
| (1,1384) | 1:18:B:VAL:HG23  | 1:59:B:ARG:HG2   | 3        | 0.63          |
| (1,1383) | 1:18:A:VAL:HG23  | 1:59:A:ARG:HG2   | 3        | 0.63          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 4        | 0.63          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 4        | 0.63          |
| (1,921)  | 1:116:A:ALA:HB3  | 1:115:A:LYS:HA   | 11       | 0.63          |
| (1,772)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HG22  | 3        | 0.63          |
| (1,772)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HG23  | 20       | 0.63          |
| (1,288)  | 1:106:B:THR:HG21 | 1:85:B:THR:HG23  | 11       | 0.63          |
| (1,287)  | 1:106:A:THR:HG21 | 1:85:A:THR:HG23  | 11       | 0.63          |
| (1,48)   | 1:42:B:VAL:HG22  | 1:44:B:ILE:HB    | 18       | 0.63          |
| (1,47)   | 1:42:A:VAL:HG22  | 1:44:A:ILE:HB    | 18       | 0.63          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG11 | 1        | 0.63          |
| (1,10)   | 1:111:B:VAL:HG23 | 1:111:B:VAL:HG11 | 13       | 0.63          |
| (1,10)   | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG12 | 15       | 0.63          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG11 | 1        | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,9)    | 1:111:A:VAL:HG23 | 1:111:A:VAL:HG11 | 13       | 0.63          |
| (1,9)    | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG12 | 15       | 0.63          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 10       | 0.62          |
| (1,3093) | 1:86:A:PHE:H     | 1:54:B:PHE:HE2   | 8        | 0.62          |
| (1,3092) | 1:86:B:PHE:H     | 1:54:A:PHE:HD1   | 13       | 0.62          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 8        | 0.62          |
| (1,3047) | 1:21:A:TRP:HZ2   | 1:31:B:ILE:HD13  | 14       | 0.62          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 4        | 0.62          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 4        | 0.62          |
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 6        | 0.62          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 6        | 0.62          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 9        | 0.62          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB3   | 7        | 0.62          |
| (1,1898) | 1:48:B:VAL:H     | 1:48:B:VAL:HG13  | 7        | 0.62          |
| (1,1872) | 1:21:B:TRP:HE1   | 1:21:B:TRP:H     | 16       | 0.62          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG23  | 10       | 0.62          |
| (1,1436) | 1:38:B:VAL:HG21  | 1:28:B:ALA:HB3   | 14       | 0.62          |
| (1,1435) | 1:38:A:VAL:HG21  | 1:28:A:ALA:HB3   | 14       | 0.62          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 20       | 0.62          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 20       | 0.62          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG11 | 15       | 0.62          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG11 | 15       | 0.62          |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB2   | 10       | 0.62          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG21  | 5        | 0.62          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG21  | 5        | 0.62          |
| (1,10)   | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG11 | 4        | 0.62          |
| (1,10)   | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG11 | 8        | 0.62          |
| (1,10)   | 1:111:B:VAL:HG23 | 1:111:B:VAL:HG13 | 9        | 0.62          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG13 | 16       | 0.62          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG11 | 18       | 0.62          |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG12 | 19       | 0.62          |
| (1,9)    | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG11 | 4        | 0.62          |
| (1,9)    | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG11 | 8        | 0.62          |
| (1,9)    | 1:111:A:VAL:HG23 | 1:111:A:VAL:HG13 | 9        | 0.62          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG11 | 18       | 0.62          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG12 | 19       | 0.62          |
| (3,8)    | 1:79:B:TYR:H     | 1:112:B:LEU:HD23 | 20       | 0.61          |
| (3,7)    | 1:79:A:TYR:H     | 1:112:A:LEU:HD23 | 20       | 0.61          |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD12  | 18       | 0.61          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 4        | 0.61          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 4        | 0.61          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 18       | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG22  | 12       | 0.61          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG23  | 13       | 0.61          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG22  | 12       | 0.61          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG23  | 13       | 0.61          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 9        | 0.61          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 7        | 0.61          |
| (1,2142) | 1:32:B:LYS:H     | 1:32:B:LYS:HG2   | 4        | 0.61          |
| (1,2142) | 1:32:B:LYS:H     | 1:32:B:LYS:HG2   | 8        | 0.61          |
| (1,2141) | 1:32:A:LYS:H     | 1:32:A:LYS:HG2   | 4        | 0.61          |
| (1,2141) | 1:32:A:LYS:H     | 1:32:A:LYS:HG2   | 8        | 0.61          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG23  | 10       | 0.61          |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB3   | 18       | 0.61          |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB3   | 18       | 0.61          |
| (1,1404) | 1:20:B:VAL:HG22  | 1:55:B:GLU:HG2   | 9        | 0.61          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 19       | 0.61          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 19       | 0.61          |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB2   | 10       | 0.61          |
| (1,416)  | 1:39:B:LEU:H     | 1:38:B:VAL:HG12  | 20       | 0.61          |
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG12  | 20       | 0.61          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG13  | 1        | 0.61          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG13  | 1        | 0.61          |
| (1,10)   | 1:111:B:VAL:HG23 | 1:111:B:VAL:HG11 | 7        | 0.61          |
| (1,9)    | 1:111:A:VAL:HG23 | 1:111:A:VAL:HG11 | 7        | 0.61          |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG13 | 16       | 0.61          |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD13  | 11       | 0.6           |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD13  | 11       | 0.6           |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 1        | 0.6           |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 1        | 0.6           |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD23 | 9        | 0.6           |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 10       | 0.6           |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD23 | 9        | 0.6           |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 15       | 0.6           |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 6        | 0.6           |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG12 | 3        | 0.6           |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG12 | 10       | 0.6           |
| (1,3060) | 1:71:B:ILE:HD12  | 1:14:A:VAL:HB    | 5        | 0.6           |
| (1,3059) | 1:71:A:ILE:HD12  | 1:14:B:VAL:HB    | 5        | 0.6           |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 18       | 0.6           |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 11       | 0.6           |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 2        | 0.6           |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 6        | 0.6           |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 6        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 14       | 0.6           |
| (1,1871) | 1:21:A:TRP:HE1   | 1:21:A:TRP:H     | 16       | 0.6           |
| (1,1208) | 1:37:B:MET:HB2   | 1:26:B:THR:HG21  | 8        | 0.6           |
| (1,1207) | 1:37:A:MET:HB2   | 1:26:A:THR:HG21  | 8        | 0.6           |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG22  | 12       | 0.6           |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23  | 10       | 0.6           |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG12  | 7        | 0.6           |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG12  | 7        | 0.6           |
| (1,10)   | 1:111:B:VAL:HG21 | 1:111:B:VAL:HG11 | 20       | 0.6           |
| (1,9)    | 1:111:A:VAL:HG21 | 1:111:A:VAL:HG11 | 20       | 0.6           |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG22 | 9        | 0.6           |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG22 | 9        | 0.6           |
| (1,3091) | 1:86:A:PHE:H     | 1:54:B:PHE:HD1   | 13       | 0.59          |
| (1,3088) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HA    | 3        | 0.59          |
| (1,3087) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HA    | 1        | 0.59          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 4        | 0.59          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG12 | 10       | 0.59          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 6        | 0.59          |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3   | 6        | 0.59          |
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 7        | 0.59          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 7        | 0.59          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 11       | 0.59          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 14       | 0.59          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 2        | 0.59          |
| (1,1430) | 1:102:B:ILE:HD12 | 1:28:B:ALA:HB1   | 15       | 0.59          |
| (1,1429) | 1:102:A:ILE:HD12 | 1:28:A:ALA:HB1   | 15       | 0.59          |
| (1,1388) | 1:20:B:VAL:HG12  | 1:19:B:SER:H     | 19       | 0.59          |
| (1,1168) | 1:92:B:MET:HE2   | 1:92:B:MET:HG2   | 19       | 0.59          |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2   | 19       | 0.59          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG22  | 12       | 0.59          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 1        | 0.59          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 1        | 0.59          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG13 | 7        | 0.59          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG13 | 7        | 0.59          |
| (1,912)  | 1:9:B:ARG:HB2    | 1:6:B:ILE:HG13   | 3        | 0.59          |
| (1,911)  | 1:9:A:ARG:HB2    | 1:6:A:ILE:HG13   | 3        | 0.59          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23  | 10       | 0.59          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG22  | 5        | 0.59          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG22  | 5        | 0.59          |
| (1,258)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HB2   | 13       | 0.59          |
| (1,257)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HB2   | 13       | 0.59          |
| (1,193)  | 1:81:A:THR:HG23  | 1:79:A:TYR:HE1   | 6        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB    | 17       | 0.59          |
| (1,10)   | 1:111:B:VAL:HG22 | 1:111:B:VAL:HG13 | 17       | 0.59          |
| (1,9)    | 1:111:A:VAL:HG22 | 1:111:A:VAL:HG13 | 17       | 0.59          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG12 | 3        | 0.58          |
| (1,3048) | 1:21:B:TRP:HZ2   | 1:31:A:ILE:HD13  | 14       | 0.58          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 16       | 0.58          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 16       | 0.58          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 14       | 0.58          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 14       | 0.58          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 16       | 0.58          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 16       | 0.58          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 16       | 0.58          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 16       | 0.58          |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2   | 8        | 0.58          |
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2   | 8        | 0.58          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG21  | 17       | 0.58          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG21  | 17       | 0.58          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG23  | 13       | 0.58          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG23  | 13       | 0.58          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG21  | 1        | 0.58          |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG21  | 14       | 0.58          |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG21  | 14       | 0.58          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 5        | 0.58          |
| (1,194)  | 1:81:B:THR:HG23  | 1:79:B:TYR:HE1   | 6        | 0.58          |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB    | 17       | 0.58          |
| (1,3087) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HA    | 3        | 0.57          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 12       | 0.57          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 4        | 0.57          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 9        | 0.57          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 9        | 0.57          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG12  | 8        | 0.57          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG12  | 8        | 0.57          |
| (1,2852) | 1:73:B:SER:H     | 1:71:B:ILE:HG21  | 1        | 0.57          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 7        | 0.57          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 20       | 0.57          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 7        | 0.57          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 20       | 0.57          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG22  | 2        | 0.57          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 11       | 0.57          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 11       | 0.57          |
| (1,1996) | 1:67:B:GLY:H     | 1:64:B:VAL:HB    | 6        | 0.57          |
| (1,1995) | 1:67:A:GLY:H     | 1:64:A:VAL:HB    | 6        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H     | 11       | 0.57          |
| (1,1387) | 1:20:A:VAL:HG12  | 1:19:A:SER:H     | 19       | 0.57          |
| (1,1168) | 1:92:B:MET:HE3   | 1:92:B:MET:HG2   | 18       | 0.57          |
| (1,596)  | 1:107:B:ALA:HB3  | 1:106:B:THR:HA   | 8        | 0.57          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 13       | 0.57          |
| (1,595)  | 1:107:A:ALA:HB3  | 1:106:A:THR:HA   | 8        | 0.57          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 13       | 0.57          |
| (1,548)  | 1:92:B:MET:HE2   | 1:92:B:MET:HB2   | 1        | 0.57          |
| (1,547)  | 1:92:A:MET:HE2   | 1:92:A:MET:HB2   | 1        | 0.57          |
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 19       | 0.57          |
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 19       | 0.57          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG22  | 11       | 0.57          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG21  | 1        | 0.57          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG22  | 11       | 0.57          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 5        | 0.57          |
| (1,3098) | 1:85:B:THR:HG22  | 1:106:A:THR:HG21 | 5        | 0.56          |
| (1,3097) | 1:85:A:THR:HG22  | 1:106:B:THR:HG21 | 5        | 0.56          |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA    | 15       | 0.56          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 12       | 0.56          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 5        | 0.56          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 10       | 0.56          |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3   | 10       | 0.56          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG11  | 15       | 0.56          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG12  | 11       | 0.56          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG12  | 11       | 0.56          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 15       | 0.56          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 15       | 0.56          |
| (1,2851) | 1:73:A:SER:H     | 1:71:A:ILE:HG21  | 1        | 0.56          |
| (1,2850) | 1:72:B:ASP:H     | 1:73:B:SER:H     | 1        | 0.56          |
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 1        | 0.56          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 1        | 0.56          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG22  | 2        | 0.56          |
| (1,2556) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HB2  | 14       | 0.56          |
| (1,2555) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HB2  | 14       | 0.56          |
| (1,2314) | 1:96:B:GLN:HE21  | 1:95:B:LYS:HA    | 12       | 0.56          |
| (1,2313) | 1:96:A:GLN:HE21  | 1:95:A:LYS:HA    | 12       | 0.56          |
| (1,1924) | 1:72:B:ASP:H     | 1:74:B:LYS:H     | 20       | 0.56          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG22  | 6        | 0.56          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG22  | 6        | 0.56          |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB2   | 16       | 0.56          |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB2   | 16       | 0.56          |
| (1,1388) | 1:20:B:VAL:HG11  | 1:19:B:SER:H     | 11       | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1167) | 1:92:A:MET:HE3   | 1:92:A:MET:HG2   | 18       | 0.56          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 8        | 0.56          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 8        | 0.56          |
| (1,988)  | 1:27:B:THR:HG22  | 1:35:B:GLU:HG3   | 5        | 0.56          |
| (1,987)  | 1:27:A:THR:HG22  | 1:35:A:GLU:HG3   | 5        | 0.56          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 10       | 0.56          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 10       | 0.56          |
| (1,676)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HE2   | 2        | 0.56          |
| (1,676)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HE2   | 13       | 0.56          |
| (1,675)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HE2   | 2        | 0.56          |
| (1,675)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HE2   | 13       | 0.56          |
| (1,662)  | 1:42:B:VAL:HG11  | 1:90:B:LEU:HG    | 7        | 0.56          |
| (1,596)  | 1:107:B:ALA:HB3  | 1:106:B:THR:HA   | 7        | 0.56          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 12       | 0.56          |
| (1,595)  | 1:107:A:ALA:HB3  | 1:106:A:THR:HA   | 7        | 0.56          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 12       | 0.56          |
| (1,547)  | 1:92:A:MET:HE3   | 1:92:A:MET:HB2   | 8        | 0.56          |
| (1,438)  | 1:74:B:LYS:HG2   | 1:74:B:LYS:HE2   | 10       | 0.56          |
| (1,437)  | 1:74:A:LYS:HG2   | 1:74:A:LYS:HE2   | 10       | 0.56          |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG23  | 20       | 0.56          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG11  | 19       | 0.56          |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG21 | 3        | 0.56          |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG21 | 3        | 0.56          |
| (1,3088) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HA    | 1        | 0.55          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 5        | 0.55          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11  | 1        | 0.55          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11  | 15       | 0.55          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 18       | 0.55          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 18       | 0.55          |
| (1,2849) | 1:72:A:ASP:H     | 1:73:A:SER:H     | 1        | 0.55          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 8        | 0.55          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 8        | 0.55          |
| (1,2298) | 1:98:B:ALA:H     | 1:97:B:ALA:HB1   | 19       | 0.55          |
| (1,2297) | 1:98:A:ALA:H     | 1:97:A:ALA:HB1   | 19       | 0.55          |
| (1,2142) | 1:32:B:LYS:H     | 1:32:B:LYS:HG2   | 7        | 0.55          |
| (1,2141) | 1:32:A:LYS:H     | 1:32:A:LYS:HG2   | 7        | 0.55          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 9        | 0.55          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 9        | 0.55          |
| (1,1923) | 1:72:A:ASP:H     | 1:74:A:LYS:H     | 20       | 0.55          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG23 | 5        | 0.55          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG23 | 5        | 0.55          |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB1   | 9        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG13  | 20       | 0.55          |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG13  | 20       | 0.55          |
| (1,1168) | 1:92:B:MET:HE3   | 1:92:B:MET:HG2   | 1        | 0.55          |
| (1,1168) | 1:92:B:MET:HE3   | 1:92:B:MET:HG2   | 3        | 0.55          |
| (1,1167) | 1:92:A:MET:HE3   | 1:92:A:MET:HG2   | 1        | 0.55          |
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2   | 10       | 0.55          |
| (1,661)  | 1:42:A:VAL:HG11  | 1:90:A:LEU:HG    | 7        | 0.55          |
| (1,548)  | 1:92:B:MET:HE3   | 1:92:B:MET:HB2   | 8        | 0.55          |
| (1,548)  | 1:92:B:MET:HE1   | 1:92:B:MET:HB2   | 19       | 0.55          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 9        | 0.55          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 9        | 0.55          |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG23  | 20       | 0.55          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG11  | 19       | 0.55          |
| (1,335)  | 1:36:A:VAL:HG11  | 1:30:A:ASP:HB2   | 4        | 0.55          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG11 | 17       | 0.54          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 17       | 0.54          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG11  | 1        | 0.54          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 12       | 0.54          |
| (1,2852) | 1:73:B:SER:H     | 1:71:B:ILE:HG21  | 4        | 0.54          |
| (1,2851) | 1:73:A:SER:H     | 1:71:A:ILE:HG21  | 4        | 0.54          |
| (1,2730) | 1:84:B:HIS:H     | 1:83:B:THR:HG21  | 14       | 0.54          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 13       | 0.54          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 18       | 0.54          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 18       | 0.54          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG21  | 16       | 0.54          |
| (1,2604) | 1:107:B:ALA:H    | 1:82:B:THR:HA    | 14       | 0.54          |
| (1,2603) | 1:107:A:ALA:H    | 1:82:A:THR:HA    | 14       | 0.54          |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB3   | 3        | 0.54          |
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB2   | 7        | 0.54          |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB2   | 7        | 0.54          |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB1   | 9        | 0.54          |
| (1,1298) | 1:36:B:VAL:HG22  | 1:91:B:THR:H     | 9        | 0.54          |
| (1,1273) | 1:71:A:ILE:HD13  | 1:68:A:CYS:HB2   | 18       | 0.54          |
| (1,1172) | 1:39:B:LEU:HD23  | 1:92:B:MET:HG2   | 18       | 0.54          |
| (1,1171) | 1:39:A:LEU:HD23  | 1:92:A:MET:HG2   | 18       | 0.54          |
| (1,1168) | 1:92:B:MET:HE3   | 1:92:B:MET:HG2   | 7        | 0.54          |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2   | 9        | 0.54          |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2   | 10       | 0.54          |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2   | 12       | 0.54          |
| (1,1167) | 1:92:A:MET:HE3   | 1:92:A:MET:HG2   | 3        | 0.54          |
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2   | 6        | 0.54          |
| (1,1167) | 1:92:A:MET:HE3   | 1:92:A:MET:HG2   | 7        | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2   | 9        | 0.54          |
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2   | 12       | 0.54          |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2   | 16       | 0.54          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 12       | 0.54          |
| (1,908)  | 1:5:B:PRO:HA     | 1:9:B:ARG:HB2    | 6        | 0.54          |
| (1,907)  | 1:5:A:PRO:HA     | 1:9:A:ARG:HB2    | 6        | 0.54          |
| (1,744)  | 1:47:B:SER:HB2   | 1:47:B:SER:HA    | 9        | 0.54          |
| (1,744)  | 1:47:B:SER:HB2   | 1:47:B:SER:HA    | 11       | 0.54          |
| (1,744)  | 1:47:B:SER:HB2   | 1:47:B:SER:HA    | 13       | 0.54          |
| (1,744)  | 1:47:B:SER:HB2   | 1:47:B:SER:HA    | 15       | 0.54          |
| (1,744)  | 1:47:B:SER:HB2   | 1:47:B:SER:HA    | 18       | 0.54          |
| (1,744)  | 1:47:B:SER:HB2   | 1:47:B:SER:HA    | 20       | 0.54          |
| (1,743)  | 1:47:A:SER:HB2   | 1:47:A:SER:HA    | 9        | 0.54          |
| (1,743)  | 1:47:A:SER:HB2   | 1:47:A:SER:HA    | 11       | 0.54          |
| (1,743)  | 1:47:A:SER:HB2   | 1:47:A:SER:HA    | 13       | 0.54          |
| (1,743)  | 1:47:A:SER:HB2   | 1:47:A:SER:HA    | 15       | 0.54          |
| (1,743)  | 1:47:A:SER:HB2   | 1:47:A:SER:HA    | 18       | 0.54          |
| (1,743)  | 1:47:A:SER:HB2   | 1:47:A:SER:HA    | 20       | 0.54          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 16       | 0.54          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 16       | 0.54          |
| (1,547)  | 1:92:A:MET:HE1   | 1:92:A:MET:HB2   | 19       | 0.54          |
| (1,542)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD11  | 20       | 0.54          |
| (1,400)  | 1:102:B:ILE:HD12 | 1:87:B:VAL:HG21  | 12       | 0.54          |
| (1,336)  | 1:36:B:VAL:HG11  | 1:30:B:ASP:HB2   | 4        | 0.54          |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3   | 17       | 0.53          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 12       | 0.53          |
| (1,2842) | 1:74:B:LYS:H     | 1:74:B:LYS:HD2   | 1        | 0.53          |
| (1,2729) | 1:84:A:HIS:H     | 1:83:A:THR:HG21  | 14       | 0.53          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 13       | 0.53          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 9        | 0.53          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 9        | 0.53          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 15       | 0.53          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 15       | 0.53          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG21  | 16       | 0.53          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 10       | 0.53          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 10       | 0.53          |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB3   | 3        | 0.53          |
| (1,2112) | 1:117:B:VAL:H    | 1:116:B:ALA:HB1  | 6        | 0.53          |
| (1,2111) | 1:117:A:VAL:H    | 1:116:A:ALA:HB1  | 6        | 0.53          |
| (1,2031) | 1:27:A:THR:H     | 1:38:A:VAL:HG22  | 12       | 0.53          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG21 | 6        | 0.53          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG21 | 6        | 0.53          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1446) | 1:25:B:LYS:HE3   | 1:25:B:LYS:HG2  | 20       | 0.53          |
| (1,1445) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HG2  | 20       | 0.53          |
| (1,1436) | 1:38:B:VAL:HG21  | 1:28:B:ALA:HB3  | 1        | 0.53          |
| (1,1435) | 1:38:A:VAL:HG21  | 1:28:A:ALA:HB3  | 1        | 0.53          |
| (1,1297) | 1:36:A:VAL:HG22  | 1:91:A:THR:H    | 9        | 0.53          |
| (1,1274) | 1:71:B:ILE:HD13  | 1:68:B:CYS:HB2  | 18       | 0.53          |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2  | 6        | 0.53          |
| (1,1168) | 1:92:B:MET:HE2   | 1:92:B:MET:HG2  | 11       | 0.53          |
| (1,1168) | 1:92:B:MET:HE2   | 1:92:B:MET:HG2  | 14       | 0.53          |
| (1,1168) | 1:92:B:MET:HE2   | 1:92:B:MET:HG2  | 16       | 0.53          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG21 | 3        | 0.53          |
| (1,1003) | 1:53:A:PHE:HB3   | 1:22:A:VAL:HG21 | 3        | 0.53          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB   | 12       | 0.53          |
| (1,541)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD11 | 20       | 0.53          |
| (1,438)  | 1:74:B:LYS:HG2   | 1:74:B:LYS:HE2  | 15       | 0.53          |
| (1,437)  | 1:74:A:LYS:HG2   | 1:74:A:LYS:HE2  | 15       | 0.53          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG22 | 1        | 0.53          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG23 | 4        | 0.53          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG21 | 19       | 0.53          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG22 | 1        | 0.53          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG23 | 4        | 0.53          |
| (1,399)  | 1:102:A:ILE:HD12 | 1:87:A:VAL:HG21 | 12       | 0.53          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG21 | 19       | 0.53          |
| (1,392)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG22 | 9        | 0.53          |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG23 | 15       | 0.53          |
| (1,391)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG22 | 9        | 0.53          |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG23 | 15       | 0.53          |
| (1,344)  | 1:48:B:VAL:HG13  | 1:41:B:GLU:HG2  | 16       | 0.53          |
| (1,343)  | 1:48:A:VAL:HG13  | 1:41:A:GLU:HG2  | 16       | 0.53          |
| (1,233)  | 1:33:A:GLY:HA2   | 1:29:A:THR:HB   | 12       | 0.53          |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG11 | 19       | 0.53          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1  | 1        | 0.52          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1  | 1        | 0.52          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11 | 9        | 0.52          |
| (1,2841) | 1:74:A:LYS:H     | 1:74:A:LYS:HD2  | 1        | 0.52          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3  | 2        | 0.52          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3  | 9        | 0.52          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3  | 9        | 0.52          |
| (1,2608) | 1:107:B:ALA:H    | 1:56:B:THR:HG21 | 6        | 0.52          |
| (1,2607) | 1:107:A:ALA:H    | 1:56:A:THR:HG21 | 6        | 0.52          |
| (1,2604) | 1:107:B:ALA:H    | 1:82:B:THR:HA   | 3        | 0.52          |
| (1,2603) | 1:107:A:ALA:H    | 1:82:A:THR:HA   | 3        | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG21 | 19       | 0.52          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG21 | 19       | 0.52          |
| (1,2168) | 1:46:B:ASN:HD21  | 1:45:B:ASN:HA    | 6        | 0.52          |
| (1,2083) | 1:88:A:LYS:H     | 1:88:A:LYS:HD2   | 10       | 0.52          |
| (1,2032) | 1:27:B:THR:H     | 1:38:B:VAL:HG22  | 12       | 0.52          |
| (1,1778) | 1:20:B:VAL:H     | 1:20:B:VAL:HG12  | 9        | 0.52          |
| (1,1777) | 1:20:A:VAL:H     | 1:20:A:VAL:HG12  | 9        | 0.52          |
| (1,1710) | 1:76:B:TRP:H     | 1:71:B:ILE:HG22  | 14       | 0.52          |
| (1,1709) | 1:76:A:TRP:H     | 1:71:A:ILE:HG22  | 14       | 0.52          |
| (1,1538) | 1:18:B:VAL:H     | 1:57:B:LYS:HG2   | 8        | 0.52          |
| (1,1537) | 1:18:A:VAL:H     | 1:57:A:LYS:HG2   | 8        | 0.52          |
| (1,1168) | 1:92:B:MET:HE2   | 1:92:B:MET:HG2   | 2        | 0.52          |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2   | 4        | 0.52          |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2   | 2        | 0.52          |
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2   | 4        | 0.52          |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2   | 11       | 0.52          |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2   | 14       | 0.52          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB3  | 3        | 0.52          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB3  | 3        | 0.52          |
| (1,676)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HE2   | 15       | 0.52          |
| (1,675)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HE2   | 15       | 0.52          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 2        | 0.52          |
| (1,550)  | 1:92:B:MET:HE1   | 1:97:B:ALA:HB3   | 8        | 0.52          |
| (1,549)  | 1:92:A:MET:HE1   | 1:97:A:ALA:HB3   | 8        | 0.52          |
| (1,294)  | 1:106:B:THR:HG23 | 1:85:B:THR:HB    | 16       | 0.52          |
| (1,293)  | 1:106:A:THR:HG23 | 1:85:A:THR:HB    | 16       | 0.52          |
| (1,234)  | 1:33:B:GLY:HA2   | 1:29:B:THR:HB    | 12       | 0.52          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG11  | 19       | 0.52          |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 11       | 0.51          |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 11       | 0.51          |
| (1,3082) | 1:12:B:PHE:H     | 1:111:A:VAL:HG21 | 16       | 0.51          |
| (1,3081) | 1:12:A:PHE:H     | 1:111:B:VAL:HG21 | 16       | 0.51          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG12  | 11       | 0.51          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11  | 19       | 0.51          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG11  | 9        | 0.51          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG12  | 11       | 0.51          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG11  | 19       | 0.51          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 10       | 0.51          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 2        | 0.51          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 10       | 0.51          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 11       | 0.51          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 13       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 11       | 0.51          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 13       | 0.51          |
| (1,2084) | 1:88:B:LYS:H     | 1:88:B:LYS:HD2   | 10       | 0.51          |
| (1,1446) | 1:25:B:LYS:HE3   | 1:25:B:LYS:HG2   | 16       | 0.51          |
| (1,1445) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HG2   | 16       | 0.51          |
| (1,1220) | 1:20:B:VAL:HG21  | 1:20:B:VAL:HB    | 10       | 0.51          |
| (1,1220) | 1:20:B:VAL:HG21  | 1:20:B:VAL:HB    | 11       | 0.51          |
| (1,1220) | 1:20:B:VAL:HG22  | 1:20:B:VAL:HB    | 16       | 0.51          |
| (1,1219) | 1:20:A:VAL:HG21  | 1:20:A:VAL:HB    | 10       | 0.51          |
| (1,1219) | 1:20:A:VAL:HG22  | 1:20:A:VAL:HB    | 11       | 0.51          |
| (1,1219) | 1:20:A:VAL:HG22  | 1:20:A:VAL:HB    | 15       | 0.51          |
| (1,1168) | 1:92:B:MET:HE2   | 1:92:B:MET:HG2   | 13       | 0.51          |
| (1,1168) | 1:92:B:MET:HE3   | 1:92:B:MET:HG2   | 17       | 0.51          |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2   | 13       | 0.51          |
| (1,1167) | 1:92:A:MET:HE3   | 1:92:A:MET:HG2   | 17       | 0.51          |
| (1,1004) | 1:53:B:PHE:HB3   | 1:22:B:VAL:HG23  | 1        | 0.51          |
| (1,924)  | 1:81:B:THR:HG22  | 1:111:B:VAL:HG11 | 3        | 0.51          |
| (1,923)  | 1:81:A:THR:HG22  | 1:111:A:VAL:HG11 | 3        | 0.51          |
| (1,676)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HE2   | 18       | 0.51          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 2        | 0.51          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 19       | 0.51          |
| (1,438)  | 1:74:B:LYS:HG2   | 1:74:B:LYS:HE2   | 9        | 0.51          |
| (1,437)  | 1:74:A:LYS:HG2   | 1:74:A:LYS:HE2   | 9        | 0.51          |
| (1,390)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG13  | 12       | 0.51          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG11  | 17       | 0.51          |
| (1,389)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG13  | 12       | 0.51          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG11  | 17       | 0.51          |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB    | 11       | 0.51          |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 11       | 0.51          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG11  | 20       | 0.51          |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG23 | 14       | 0.51          |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG23 | 14       | 0.51          |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 12       | 0.5           |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG13 | 17       | 0.5           |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG13  | 12       | 0.5           |
| (1,2844) | 1:74:B:LYS:H     | 1:72:B:ASP:HB2   | 5        | 0.5           |
| (1,2843) | 1:74:A:LYS:H     | 1:72:A:ASP:HB2   | 5        | 0.5           |
| (1,2730) | 1:84:B:HIS:H     | 1:83:B:THR:HG21  | 5        | 0.5           |
| (1,2729) | 1:84:A:HIS:H     | 1:83:A:THR:HG21  | 5        | 0.5           |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 19       | 0.5           |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 19       | 0.5           |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 3        | 0.5           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2255) | 1:77:A:ASN:HD22 | 1:115:A:LYS:HG2  | 20       | 0.5           |
| (1,2232) | 1:118:B:ARG:H   | 1:117:B:VAL:HG11 | 10       | 0.5           |
| (1,2231) | 1:118:A:ARG:H   | 1:117:A:VAL:HG11 | 10       | 0.5           |
| (1,2186) | 1:100:B:ARG:H   | 1:98:B:ALA:HB3   | 6        | 0.5           |
| (1,2185) | 1:100:A:ARG:H   | 1:98:A:ALA:HB3   | 6        | 0.5           |
| (1,1871) | 1:21:A:TRP:HE1  | 1:21:A:TRP:H     | 20       | 0.5           |
| (1,1537) | 1:18:A:VAL:H    | 1:57:A:LYS:HG2   | 10       | 0.5           |
| (1,1446) | 1:25:B:LYS:HE3  | 1:25:B:LYS:HG2   | 19       | 0.5           |
| (1,1445) | 1:25:A:LYS:HE3  | 1:25:A:LYS:HG2   | 19       | 0.5           |
| (1,1436) | 1:38:B:VAL:HG23 | 1:28:B:ALA:HB3   | 18       | 0.5           |
| (1,1435) | 1:38:A:VAL:HG23 | 1:28:A:ALA:HB3   | 18       | 0.5           |
| (1,1248) | 1:71:B:ILE:HG12 | 1:70:B:GLY:HA3   | 4        | 0.5           |
| (1,1220) | 1:20:B:VAL:HG22 | 1:20:B:VAL:HB    | 4        | 0.5           |
| (1,1220) | 1:20:B:VAL:HG21 | 1:20:B:VAL:HB    | 5        | 0.5           |
| (1,1220) | 1:20:B:VAL:HG23 | 1:20:B:VAL:HB    | 6        | 0.5           |
| (1,1220) | 1:20:B:VAL:HG22 | 1:20:B:VAL:HB    | 7        | 0.5           |
| (1,1220) | 1:20:B:VAL:HG21 | 1:20:B:VAL:HB    | 8        | 0.5           |
| (1,1220) | 1:20:B:VAL:HG23 | 1:20:B:VAL:HB    | 14       | 0.5           |
| (1,1220) | 1:20:B:VAL:HG22 | 1:20:B:VAL:HB    | 15       | 0.5           |
| (1,1220) | 1:20:B:VAL:HG22 | 1:20:B:VAL:HB    | 19       | 0.5           |
| (1,1220) | 1:20:B:VAL:HG21 | 1:20:B:VAL:HB    | 20       | 0.5           |
| (1,1219) | 1:20:A:VAL:HG21 | 1:20:A:VAL:HB    | 3        | 0.5           |
| (1,1219) | 1:20:A:VAL:HG22 | 1:20:A:VAL:HB    | 4        | 0.5           |
| (1,1219) | 1:20:A:VAL:HG21 | 1:20:A:VAL:HB    | 5        | 0.5           |
| (1,1219) | 1:20:A:VAL:HG23 | 1:20:A:VAL:HB    | 6        | 0.5           |
| (1,1219) | 1:20:A:VAL:HG22 | 1:20:A:VAL:HB    | 7        | 0.5           |
| (1,1219) | 1:20:A:VAL:HG21 | 1:20:A:VAL:HB    | 8        | 0.5           |
| (1,1219) | 1:20:A:VAL:HG21 | 1:20:A:VAL:HB    | 14       | 0.5           |
| (1,1219) | 1:20:A:VAL:HG22 | 1:20:A:VAL:HB    | 16       | 0.5           |
| (1,1219) | 1:20:A:VAL:HG22 | 1:20:A:VAL:HB    | 19       | 0.5           |
| (1,1219) | 1:20:A:VAL:HG21 | 1:20:A:VAL:HB    | 20       | 0.5           |
| (1,1216) | 1:22:B:VAL:HG11 | 1:20:B:VAL:HB    | 13       | 0.5           |
| (1,1215) | 1:22:A:VAL:HG11 | 1:20:A:VAL:HB    | 13       | 0.5           |
| (1,1003) | 1:53:A:PHE:HB3  | 1:22:A:VAL:HG23  | 1        | 0.5           |
| (1,960)  | 1:59:B:ARG:HD2  | 1:18:B:VAL:HB    | 17       | 0.5           |
| (1,920)  | 1:117:B:VAL:HB  | 1:116:B:ALA:HB3  | 2        | 0.5           |
| (1,810)  | 1:118:B:ARG:HB2 | 1:118:B:ARG:HG2  | 14       | 0.5           |
| (1,809)  | 1:118:A:ARG:HB2 | 1:118:A:ARG:HG2  | 14       | 0.5           |
| (1,675)  | 1:34:A:LYS:HG3  | 1:34:A:LYS:HE2   | 18       | 0.5           |
| (1,583)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HD2  | 19       | 0.5           |
| (1,440)  | 1:88:B:LYS:HA   | 1:88:B:LYS:HE2   | 16       | 0.5           |
| (1,439)  | 1:88:A:LYS:HA   | 1:88:A:LYS:HE2   | 16       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG22  | 3        | 0.5           |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG22  | 16       | 0.5           |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG23  | 18       | 0.5           |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG22  | 3        | 0.5           |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG22  | 16       | 0.5           |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG23  | 18       | 0.5           |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB    | 2        | 0.5           |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB    | 4        | 0.5           |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB    | 8        | 0.5           |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB    | 13       | 0.5           |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB    | 15       | 0.5           |
| (1,350)  | 1:48:B:VAL:HG11  | 1:48:B:VAL:HB    | 19       | 0.5           |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB    | 20       | 0.5           |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 2        | 0.5           |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB    | 3        | 0.5           |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 4        | 0.5           |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 6        | 0.5           |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 8        | 0.5           |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB    | 13       | 0.5           |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 16       | 0.5           |
| (1,349)  | 1:48:A:VAL:HG11  | 1:48:A:VAL:HB    | 19       | 0.5           |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB    | 20       | 0.5           |
| (1,288)  | 1:106:B:THR:HG21 | 1:85:B:THR:HG22  | 5        | 0.5           |
| (1,287)  | 1:106:A:THR:HG21 | 1:85:A:THR:HG22  | 5        | 0.5           |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG11  | 20       | 0.5           |
| (1,47)   | 1:42:A:VAL:HG22  | 1:44:A:ILE:HB    | 5        | 0.5           |
| (1,3082) | 1:12:B:PHE:H     | 1:111:A:VAL:HG21 | 20       | 0.49          |
| (1,3076) | 1:42:B:VAL:HG22  | 1:99:A:TRP:HE1   | 5        | 0.49          |
| (1,3076) | 1:42:B:VAL:HG23  | 1:99:A:TRP:HE1   | 12       | 0.49          |
| (1,3075) | 1:42:A:VAL:HG23  | 1:99:B:TRP:HE1   | 12       | 0.49          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG12  | 18       | 0.49          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG13  | 12       | 0.49          |
| (1,2730) | 1:84:B:HIS:H     | 1:83:B:THR:HG23  | 11       | 0.49          |
| (1,2729) | 1:84:A:HIS:H     | 1:83:A:THR:HG23  | 11       | 0.49          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 14       | 0.49          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 14       | 0.49          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 1        | 0.49          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 4        | 0.49          |
| (1,2658) | 1:34:B:LYS:H     | 1:34:B:LYS:HG3   | 19       | 0.49          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 1        | 0.49          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 4        | 0.49          |
| (1,2657) | 1:34:A:LYS:H     | 1:34:A:LYS:HG3   | 19       | 0.49          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2614) | 1:19:B:SER:H    | 1:18:B:VAL:HG23  | 19       | 0.49          |
| (1,2390) | 1:29:B:THR:H    | 1:102:B:ILE:HG23 | 3        | 0.49          |
| (1,2389) | 1:29:A:THR:H    | 1:102:A:ILE:HG22 | 4        | 0.49          |
| (1,2256) | 1:77:B:ASN:HD22 | 1:115:B:LYS:HG2  | 20       | 0.49          |
| (1,2232) | 1:118:B:ARG:H   | 1:117:B:VAL:HG13 | 15       | 0.49          |
| (1,2224) | 1:118:B:ARG:H   | 1:118:B:ARG:HB2  | 14       | 0.49          |
| (1,2222) | 1:118:B:ARG:H   | 1:117:B:VAL:HB   | 1        | 0.49          |
| (1,2221) | 1:118:A:ARG:H   | 1:117:A:VAL:HB   | 1        | 0.49          |
| (1,2167) | 1:46:A:ASN:HD21 | 1:45:A:ASN:HA    | 6        | 0.49          |
| (1,2014) | 1:79:B:TYR:H    | 1:111:B:VAL:HB   | 9        | 0.49          |
| (1,2013) | 1:79:A:TYR:H    | 1:111:A:VAL:HB   | 9        | 0.49          |
| (1,1872) | 1:21:B:TRP:HE1  | 1:21:B:TRP:H     | 20       | 0.49          |
| (1,1542) | 1:54:B:PHE:HB2  | 1:55:B:GLU:HG3   | 3        | 0.49          |
| (1,1541) | 1:54:A:PHE:HB2  | 1:55:A:GLU:HG3   | 3        | 0.49          |
| (1,1538) | 1:18:B:VAL:H    | 1:57:B:LYS:HG2   | 10       | 0.49          |
| (1,1442) | 1:25:B:LYS:HG2  | 1:53:B:PHE:HD1   | 2        | 0.49          |
| (1,1441) | 1:25:A:LYS:HG2  | 1:53:A:PHE:HD1   | 2        | 0.49          |
| (1,1388) | 1:20:B:VAL:HG11 | 1:19:B:SER:H     | 13       | 0.49          |
| (1,1388) | 1:20:B:VAL:HG13 | 1:19:B:SER:H     | 16       | 0.49          |
| (1,1387) | 1:20:A:VAL:HG13 | 1:19:A:SER:H     | 12       | 0.49          |
| (1,1247) | 1:71:A:ILE:HG12 | 1:70:A:GLY:HA3   | 4        | 0.49          |
| (1,1220) | 1:20:B:VAL:HG22 | 1:20:B:VAL:HB    | 1        | 0.49          |
| (1,1220) | 1:20:B:VAL:HG21 | 1:20:B:VAL:HB    | 2        | 0.49          |
| (1,1220) | 1:20:B:VAL:HG21 | 1:20:B:VAL:HB    | 3        | 0.49          |
| (1,1220) | 1:20:B:VAL:HG22 | 1:20:B:VAL:HB    | 9        | 0.49          |
| (1,1220) | 1:20:B:VAL:HG23 | 1:20:B:VAL:HB    | 12       | 0.49          |
| (1,1220) | 1:20:B:VAL:HG23 | 1:20:B:VAL:HB    | 13       | 0.49          |
| (1,1220) | 1:20:B:VAL:HG22 | 1:20:B:VAL:HB    | 17       | 0.49          |
| (1,1220) | 1:20:B:VAL:HG23 | 1:20:B:VAL:HB    | 18       | 0.49          |
| (1,1219) | 1:20:A:VAL:HG21 | 1:20:A:VAL:HB    | 2        | 0.49          |
| (1,1219) | 1:20:A:VAL:HG22 | 1:20:A:VAL:HB    | 9        | 0.49          |
| (1,1219) | 1:20:A:VAL:HG23 | 1:20:A:VAL:HB    | 12       | 0.49          |
| (1,1219) | 1:20:A:VAL:HG23 | 1:20:A:VAL:HB    | 13       | 0.49          |
| (1,1219) | 1:20:A:VAL:HG22 | 1:20:A:VAL:HB    | 17       | 0.49          |
| (1,1219) | 1:20:A:VAL:HG23 | 1:20:A:VAL:HB    | 18       | 0.49          |
| (1,1171) | 1:39:A:LEU:HD22 | 1:92:A:MET:HG2   | 17       | 0.49          |
| (1,1017) | 1:18:A:VAL:HG23 | 1:18:A:VAL:HB    | 7        | 0.49          |
| (1,959)  | 1:59:A:ARG:HD2  | 1:18:A:VAL:HB    | 17       | 0.49          |
| (1,919)  | 1:117:A:VAL:HB  | 1:116:A:ALA:HB3  | 2        | 0.49          |
| (1,588)  | 1:115:B:LYS:HD2 | 1:115:B:LYS:HB3  | 2        | 0.49          |
| (1,587)  | 1:115:A:LYS:HD2 | 1:115:A:LYS:HB3  | 2        | 0.49          |
| (1,554)  | 1:88:B:LYS:HG2  | 1:88:B:LYS:HE2   | 9        | 0.49          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,553)  | 1:88:A:LYS:HG2   | 1:88:A:LYS:HE2  | 9        | 0.49          |
| (1,542)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD12 | 3        | 0.49          |
| (1,402)  | 1:102:B:ILE:HD12 | 1:25:B:LYS:HG2  | 16       | 0.49          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG21 | 6        | 0.49          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG22 | 15       | 0.49          |
| (1,400)  | 1:102:B:ILE:HD11 | 1:87:B:VAL:HG21 | 17       | 0.49          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG21 | 6        | 0.49          |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG22 | 15       | 0.49          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG23 | 4        | 0.49          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG23 | 4        | 0.49          |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB   | 3        | 0.49          |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB   | 5        | 0.49          |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB   | 6        | 0.49          |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB   | 9        | 0.49          |
| (1,350)  | 1:48:B:VAL:HG11  | 1:48:B:VAL:HB   | 10       | 0.49          |
| (1,350)  | 1:48:B:VAL:HG11  | 1:48:B:VAL:HB   | 12       | 0.49          |
| (1,350)  | 1:48:B:VAL:HG11  | 1:48:B:VAL:HB   | 14       | 0.49          |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB   | 16       | 0.49          |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB   | 17       | 0.49          |
| (1,350)  | 1:48:B:VAL:HG12  | 1:48:B:VAL:HB   | 18       | 0.49          |
| (1,349)  | 1:48:A:VAL:HG11  | 1:48:A:VAL:HB   | 7        | 0.49          |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB   | 9        | 0.49          |
| (1,349)  | 1:48:A:VAL:HG11  | 1:48:A:VAL:HB   | 10       | 0.49          |
| (1,349)  | 1:48:A:VAL:HG11  | 1:48:A:VAL:HB   | 12       | 0.49          |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB   | 15       | 0.49          |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB   | 17       | 0.49          |
| (1,349)  | 1:48:A:VAL:HG12  | 1:48:A:VAL:HB   | 18       | 0.49          |
| (1,336)  | 1:36:B:VAL:HG13  | 1:30:B:ASP:HB2  | 3        | 0.49          |
| (1,335)  | 1:36:A:VAL:HG13  | 1:30:A:ASP:HB2  | 3        | 0.49          |
| (1,158)  | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2  | 14       | 0.49          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2  | 14       | 0.49          |
| (1,48)   | 1:42:B:VAL:HG22  | 1:44:B:ILE:HB   | 5        | 0.49          |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA   | 12       | 0.48          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA  | 7        | 0.48          |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA  | 7        | 0.48          |
| (1,3075) | 1:42:A:VAL:HG22  | 1:99:B:TRP:HE1  | 5        | 0.48          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3  | 16       | 0.48          |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3  | 16       | 0.48          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG12 | 5        | 0.48          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG12 | 18       | 0.48          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG12 | 5        | 0.48          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3  | 6        | 0.48          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2853) | 1:73:A:SER:H    | 1:76:A:TRP:HB3   | 6        | 0.48          |
| (1,2658) | 1:34:B:LYS:H    | 1:34:B:LYS:HG3   | 5        | 0.48          |
| (1,2657) | 1:34:A:LYS:H    | 1:34:A:LYS:HG3   | 5        | 0.48          |
| (1,2613) | 1:19:A:SER:H    | 1:18:A:VAL:HG23  | 19       | 0.48          |
| (1,2544) | 1:76:B:TRP:HE1  | 1:112:B:LEU:HD23 | 8        | 0.48          |
| (1,2390) | 1:29:B:THR:H    | 1:102:B:ILE:HG22 | 4        | 0.48          |
| (1,2231) | 1:118:A:ARG:H   | 1:117:A:VAL:HG13 | 15       | 0.48          |
| (1,2223) | 1:118:A:ARG:H   | 1:118:A:ARG:HB2  | 14       | 0.48          |
| (1,2222) | 1:118:B:ARG:H   | 1:117:B:VAL:HB   | 13       | 0.48          |
| (1,2221) | 1:118:A:ARG:H   | 1:117:A:VAL:HB   | 13       | 0.48          |
| (1,1446) | 1:25:B:LYS:HE3  | 1:25:B:LYS:HG2   | 2        | 0.48          |
| (1,1445) | 1:25:A:LYS:HE3  | 1:25:A:LYS:HG2   | 2        | 0.48          |
| (1,1388) | 1:20:B:VAL:HG13 | 1:19:B:SER:H     | 12       | 0.48          |
| (1,1387) | 1:20:A:VAL:HG13 | 1:19:A:SER:H     | 16       | 0.48          |
| (1,1219) | 1:20:A:VAL:HG22 | 1:20:A:VAL:HB    | 1        | 0.48          |
| (1,1172) | 1:39:B:LEU:HD23 | 1:92:B:MET:HG2   | 2        | 0.48          |
| (1,1172) | 1:39:B:LEU:HD22 | 1:92:B:MET:HG2   | 17       | 0.48          |
| (1,1171) | 1:39:A:LEU:HD23 | 1:92:A:MET:HG2   | 2        | 0.48          |
| (1,1168) | 1:92:B:MET:HE2  | 1:92:B:MET:HG2   | 20       | 0.48          |
| (1,1028) | 1:18:B:VAL:HA   | 1:19:B:SER:HB2   | 5        | 0.48          |
| (1,1027) | 1:18:A:VAL:HA   | 1:19:A:SER:HB2   | 5        | 0.48          |
| (1,1018) | 1:18:B:VAL:HG22 | 1:18:B:VAL:HB    | 1        | 0.48          |
| (1,1018) | 1:18:B:VAL:HG22 | 1:18:B:VAL:HB    | 3        | 0.48          |
| (1,1018) | 1:18:B:VAL:HG22 | 1:18:B:VAL:HB    | 5        | 0.48          |
| (1,1018) | 1:18:B:VAL:HG22 | 1:18:B:VAL:HB    | 6        | 0.48          |
| (1,1018) | 1:18:B:VAL:HG23 | 1:18:B:VAL:HB    | 7        | 0.48          |
| (1,1018) | 1:18:B:VAL:HG23 | 1:18:B:VAL:HB    | 8        | 0.48          |
| (1,1018) | 1:18:B:VAL:HG21 | 1:18:B:VAL:HB    | 10       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG22 | 1:18:B:VAL:HB    | 12       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG23 | 1:18:B:VAL:HB    | 13       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG21 | 1:18:B:VAL:HB    | 14       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG21 | 1:18:B:VAL:HB    | 15       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG21 | 1:18:B:VAL:HB    | 16       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG23 | 1:18:B:VAL:HB    | 17       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG21 | 1:18:B:VAL:HB    | 18       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG22 | 1:18:B:VAL:HB    | 19       | 0.48          |
| (1,1018) | 1:18:B:VAL:HG23 | 1:18:B:VAL:HB    | 20       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG22 | 1:18:A:VAL:HB    | 1        | 0.48          |
| (1,1017) | 1:18:A:VAL:HG22 | 1:18:A:VAL:HB    | 3        | 0.48          |
| (1,1017) | 1:18:A:VAL:HG21 | 1:18:A:VAL:HB    | 4        | 0.48          |
| (1,1017) | 1:18:A:VAL:HG22 | 1:18:A:VAL:HB    | 5        | 0.48          |
| (1,1017) | 1:18:A:VAL:HG22 | 1:18:A:VAL:HB    | 6        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1017) | 1:18:A:VAL:HG23  | 1:18:A:VAL:HB    | 8        | 0.48          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 10       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG22  | 1:18:A:VAL:HB    | 12       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG23  | 1:18:A:VAL:HB    | 13       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 14       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 15       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 16       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG23  | 1:18:A:VAL:HB    | 17       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 18       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG22  | 1:18:A:VAL:HB    | 19       | 0.48          |
| (1,1017) | 1:18:A:VAL:HG23  | 1:18:A:VAL:HB    | 20       | 0.48          |
| (1,662)  | 1:42:B:VAL:HG11  | 1:90:B:LEU:HG    | 9        | 0.48          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 20       | 0.48          |
| (1,661)  | 1:42:A:VAL:HG11  | 1:90:A:LEU:HG    | 9        | 0.48          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 20       | 0.48          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 10       | 0.48          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 17       | 0.48          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 10       | 0.48          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 18       | 0.48          |
| (1,541)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD12  | 3        | 0.48          |
| (1,401)  | 1:102:A:ILE:HD12 | 1:25:A:LYS:HG2   | 16       | 0.48          |
| (1,399)  | 1:102:A:ILE:HD11 | 1:87:A:VAL:HG21  | 17       | 0.48          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG21  | 13       | 0.48          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG21  | 13       | 0.48          |
| (1,350)  | 1:48:B:VAL:HG11  | 1:48:B:VAL:HB    | 7        | 0.48          |
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 5        | 0.48          |
| (1,349)  | 1:48:A:VAL:HG11  | 1:48:A:VAL:HB    | 14       | 0.48          |
| (1,336)  | 1:36:B:VAL:HG12  | 1:30:B:ASP:HB2   | 14       | 0.48          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 18       | 0.47          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB3  | 14       | 0.47          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB3  | 14       | 0.47          |
| (1,3060) | 1:71:B:ILE:HD12  | 1:14:A:VAL:HB    | 13       | 0.47          |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD23 | 8        | 0.47          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2  | 12       | 0.47          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 12       | 0.47          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3  | 17       | 0.47          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3  | 17       | 0.47          |
| (1,1872) | 1:21:B:TRP:HE1   | 1:21:B:TRP:H     | 6        | 0.47          |
| (1,1871) | 1:21:A:TRP:HE1   | 1:21:A:TRP:H     | 6        | 0.47          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG12  | 11       | 0.47          |
| (1,1486) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HG22  | 10       | 0.47          |
| (1,1485) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HG22  | 10       | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1436) | 1:38:B:VAL:HG22  | 1:28:B:ALA:HB3   | 2        | 0.47          |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB2   | 4        | 0.47          |
| (1,1435) | 1:38:A:VAL:HG22  | 1:28:A:ALA:HB3   | 2        | 0.47          |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB2   | 4        | 0.47          |
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H     | 13       | 0.47          |
| (1,1384) | 1:18:B:VAL:HG21  | 1:59:B:ARG:HG2   | 17       | 0.47          |
| (1,1203) | 1:37:A:MET:HE3   | 1:26:A:THR:HG21  | 14       | 0.47          |
| (1,1168) | 1:92:B:MET:HE1   | 1:92:B:MET:HG2   | 5        | 0.47          |
| (1,1167) | 1:92:A:MET:HE1   | 1:92:A:MET:HG2   | 5        | 0.47          |
| (1,1167) | 1:92:A:MET:HE2   | 1:92:A:MET:HG2   | 20       | 0.47          |
| (1,1027) | 1:18:A:VAL:HA    | 1:19:A:SER:HB2   | 3        | 0.47          |
| (1,1018) | 1:18:B:VAL:HG21  | 1:18:B:VAL:HB    | 2        | 0.47          |
| (1,1018) | 1:18:B:VAL:HG21  | 1:18:B:VAL:HB    | 4        | 0.47          |
| (1,1018) | 1:18:B:VAL:HG21  | 1:18:B:VAL:HB    | 9        | 0.47          |
| (1,1018) | 1:18:B:VAL:HG21  | 1:18:B:VAL:HB    | 11       | 0.47          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 2        | 0.47          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 9        | 0.47          |
| (1,1017) | 1:18:A:VAL:HG21  | 1:18:A:VAL:HB    | 11       | 0.47          |
| (1,924)  | 1:81:B:THR:HG21  | 1:111:B:VAL:HG13 | 4        | 0.47          |
| (1,924)  | 1:81:B:THR:HG23  | 1:111:B:VAL:HG11 | 6        | 0.47          |
| (1,923)  | 1:81:A:THR:HG21  | 1:111:A:VAL:HG13 | 4        | 0.47          |
| (1,923)  | 1:81:A:THR:HG23  | 1:111:A:VAL:HG11 | 6        | 0.47          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB3  | 5        | 0.47          |
| (1,676)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HE2   | 14       | 0.47          |
| (1,675)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HE2   | 14       | 0.47          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 1        | 0.47          |
| (1,596)  | 1:107:B:ALA:HB2  | 1:106:B:THR:HA   | 2        | 0.47          |
| (1,596)  | 1:107:B:ALA:HB2  | 1:106:B:THR:HA   | 18       | 0.47          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 1        | 0.47          |
| (1,595)  | 1:107:A:ALA:HB2  | 1:106:A:THR:HA   | 2        | 0.47          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 17       | 0.47          |
| (1,595)  | 1:107:A:ALA:HB2  | 1:106:A:THR:HA   | 18       | 0.47          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 18       | 0.47          |
| (1,549)  | 1:92:A:MET:HE3   | 1:97:A:ALA:HB1   | 20       | 0.47          |
| (1,392)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG22  | 2        | 0.47          |
| (1,391)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG22  | 2        | 0.47          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD12 | 3        | 0.47          |
| (1,384)  | 1:104:B:ILE:HG22 | 1:104:B:ILE:HD13 | 15       | 0.47          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD12 | 3        | 0.47          |
| (1,383)  | 1:104:A:ILE:HG22 | 1:104:A:ILE:HD11 | 5        | 0.47          |
| (1,383)  | 1:104:A:ILE:HG22 | 1:104:A:ILE:HD13 | 15       | 0.47          |
| (1,350)  | 1:48:B:VAL:HG13  | 1:48:B:VAL:HB    | 1        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,349)  | 1:48:A:VAL:HG13  | 1:48:A:VAL:HB    | 1        | 0.47          |
| (1,335)  | 1:36:A:VAL:HG12  | 1:30:A:ASP:HB2   | 14       | 0.47          |
| (1,270)  | 1:14:B:VAL:HG12  | 1:110:B:CYS:HB3  | 6        | 0.47          |
| (1,269)  | 1:14:A:VAL:HG12  | 1:110:A:CYS:HB3  | 6        | 0.47          |
| (1,48)   | 1:42:B:VAL:HG21  | 1:44:B:ILE:HB    | 20       | 0.47          |
| (1,47)   | 1:42:A:VAL:HG21  | 1:44:A:ILE:HB    | 20       | 0.47          |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD12  | 1        | 0.46          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD12  | 1        | 0.46          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 3        | 0.46          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 3        | 0.46          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 20       | 0.46          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 8        | 0.46          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 8        | 0.46          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 10       | 0.46          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 10       | 0.46          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 19       | 0.46          |
| (1,1649) | 1:47:A:SER:H     | 1:48:A:VAL:HG12  | 11       | 0.46          |
| (1,1436) | 1:38:B:VAL:HG21  | 1:28:B:ALA:HB3   | 17       | 0.46          |
| (1,1435) | 1:38:A:VAL:HG21  | 1:28:A:ALA:HB3   | 17       | 0.46          |
| (1,1383) | 1:18:A:VAL:HG21  | 1:59:A:ARG:HG2   | 17       | 0.46          |
| (1,1298) | 1:36:B:VAL:HG23  | 1:91:B:THR:H     | 12       | 0.46          |
| (1,1297) | 1:36:A:VAL:HG23  | 1:91:A:THR:H     | 12       | 0.46          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 1        | 0.46          |
| (1,1247) | 1:71:A:ILE:HG12  | 1:70:A:GLY:HA3   | 1        | 0.46          |
| (1,1204) | 1:37:B:MET:HE3   | 1:26:B:THR:HG21  | 14       | 0.46          |
| (1,1028) | 1:18:B:VAL:HA    | 1:19:B:SER:HB2   | 3        | 0.46          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB3  | 5        | 0.46          |
| (1,596)  | 1:107:B:ALA:HB3  | 1:106:B:THR:HA   | 6        | 0.46          |
| (1,595)  | 1:107:A:ALA:HB3  | 1:106:A:THR:HA   | 6        | 0.46          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 13       | 0.46          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 13       | 0.46          |
| (1,550)  | 1:92:B:MET:HE3   | 1:97:B:ALA:HB1   | 20       | 0.46          |
| (1,549)  | 1:92:A:MET:HE2   | 1:97:A:ALA:HB2   | 12       | 0.46          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG22  | 19       | 0.46          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG22  | 19       | 0.46          |
| (1,390)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG13  | 4        | 0.46          |
| (1,389)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG13  | 4        | 0.46          |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG13  | 20       | 0.46          |
| (1,384)  | 1:104:B:ILE:HG22 | 1:104:B:ILE:HD11 | 5        | 0.46          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD13 | 19       | 0.46          |
| (1,336)  | 1:36:B:VAL:HG13  | 1:30:B:ASP:HB2   | 1        | 0.46          |
| (1,335)  | 1:36:A:VAL:HG13  | 1:30:A:ASP:HB2   | 1        | 0.46          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,258)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HB2  | 11       | 0.46          |
| (1,257)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HB2  | 11       | 0.46          |
| (1,250)  | 1:112:B:LEU:HD21 | 1:76:B:TRP:HD1  | 14       | 0.46          |
| (1,158)  | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2  | 10       | 0.46          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2  | 10       | 0.46          |
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB   | 1        | 0.46          |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB   | 1        | 0.46          |
| (1,3085) | 1:112:A:LEU:HD12 | 1:14:B:VAL:HG22 | 6        | 0.45          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3  | 6        | 0.45          |
| (1,2842) | 1:74:B:LYS:H     | 1:74:B:LYS:HD2  | 7        | 0.45          |
| (1,2841) | 1:74:A:LYS:H     | 1:74:A:LYS:HD2  | 7        | 0.45          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3 | 17       | 0.45          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3 | 17       | 0.45          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3  | 4        | 0.45          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3  | 4        | 0.45          |
| (1,2314) | 1:96:B:GLN:HE21  | 1:95:B:LYS:HA   | 17       | 0.45          |
| (1,2313) | 1:96:A:GLN:HE21  | 1:95:A:LYS:HA   | 17       | 0.45          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA  | 20       | 0.45          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA  | 12       | 0.45          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA  | 14       | 0.45          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA  | 15       | 0.45          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA  | 12       | 0.45          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA  | 14       | 0.45          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2 | 9        | 0.45          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB  | 6        | 0.45          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB  | 6        | 0.45          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB  | 18       | 0.45          |
| (1,2196) | 1:55:B:GLU:H     | 1:22:B:VAL:HG11 | 8        | 0.45          |
| (1,2195) | 1:55:A:GLU:H     | 1:22:A:VAL:HG11 | 8        | 0.45          |
| (1,2176) | 1:100:B:ARG:H    | 1:100:B:ARG:HG3 | 18       | 0.45          |
| (1,2175) | 1:100:A:ARG:H    | 1:100:A:ARG:HG3 | 18       | 0.45          |
| (1,2152) | 1:77:B:ASN:H     | 1:115:B:LYS:HD2 | 17       | 0.45          |
| (1,2151) | 1:77:A:ASN:H     | 1:115:A:LYS:HD2 | 17       | 0.45          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB   | 19       | 0.45          |
| (1,2001) | 1:79:A:TYR:H     | 1:111:A:VAL:HA  | 17       | 0.45          |
| (1,1445) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HG2  | 3        | 0.45          |
| (1,1445) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HG2  | 13       | 0.45          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1  | 16       | 0.45          |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG13 | 6        | 0.45          |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG13 | 6        | 0.45          |
| (1,554)  | 1:88:B:LYS:HG2   | 1:88:B:LYS:HE2  | 4        | 0.45          |
| (1,553)  | 1:88:A:LYS:HG2   | 1:88:A:LYS:HE2  | 4        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,553)  | 1:88:A:LYS:HG2   | 1:88:A:LYS:HE2   | 11       | 0.45          |
| (1,550)  | 1:92:B:MET:HE2   | 1:97:B:ALA:HB2   | 12       | 0.45          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 3        | 0.45          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 3        | 0.45          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG23  | 14       | 0.45          |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG23  | 14       | 0.45          |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG23  | 8        | 0.45          |
| (1,392)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG23  | 10       | 0.45          |
| (1,392)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG21  | 12       | 0.45          |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG23  | 8        | 0.45          |
| (1,391)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG23  | 10       | 0.45          |
| (1,391)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG21  | 12       | 0.45          |
| (1,390)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG13  | 10       | 0.45          |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG13  | 20       | 0.45          |
| (1,389)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG13  | 10       | 0.45          |
| (1,389)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG11  | 16       | 0.45          |
| (1,384)  | 1:104:B:ILE:HG22 | 1:104:B:ILE:HD13 | 1        | 0.45          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD12 | 10       | 0.45          |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD12 | 13       | 0.45          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD13 | 19       | 0.45          |
| (1,383)  | 1:104:A:ILE:HG22 | 1:104:A:ILE:HD13 | 1        | 0.45          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD12 | 8        | 0.45          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD12 | 10       | 0.45          |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD12 | 13       | 0.45          |
| (1,249)  | 1:112:A:LEU:HD21 | 1:76:A:TRP:HD1   | 14       | 0.45          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 20       | 0.45          |
| (1,184)  | 1:94:B:GLY:HA2   | 1:95:B:LYS:HB2   | 7        | 0.45          |
| (1,183)  | 1:94:A:GLY:HA2   | 1:95:A:LYS:HB2   | 7        | 0.45          |
| (1,158)  | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2   | 18       | 0.45          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2   | 2        | 0.45          |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG23 | 2        | 0.45          |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG23 | 2        | 0.45          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 3        | 0.44          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD21 | 3        | 0.44          |
| (1,3094) | 1:86:B:PHE:H     | 1:54:A:PHE:HE1   | 5        | 0.44          |
| (1,3093) | 1:86:A:PHE:H     | 1:54:B:PHE:HE1   | 5        | 0.44          |
| (1,3090) | 1:112:B:LEU:HD22 | 1:14:A:VAL:HA    | 2        | 0.44          |
| (1,3081) | 1:12:A:PHE:H     | 1:111:B:VAL:HG21 | 20       | 0.44          |
| (1,3075) | 1:42:A:VAL:HG23  | 1:99:B:TRP:HE1   | 7        | 0.44          |
| (1,3052) | 1:21:B:TRP:HE1   | 1:31:A:ILE:HD12  | 16       | 0.44          |
| (1,3051) | 1:21:A:TRP:HE1   | 1:31:B:ILE:HD12  | 16       | 0.44          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11  | 13       | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG11  | 13       | 0.44          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 6        | 0.44          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 17       | 0.44          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 17       | 0.44          |
| (1,2736) | 1:51:B:GLN:HE21  | 1:90:B:LEU:H     | 10       | 0.44          |
| (1,2603) | 1:107:A:ALA:H    | 1:82:A:THR:HA    | 11       | 0.44          |
| (1,2584) | 1:107:B:ALA:H    | 1:83:B:THR:HB    | 3        | 0.44          |
| (1,2583) | 1:107:A:ALA:H    | 1:83:A:THR:HB    | 3        | 0.44          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 16       | 0.44          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 18       | 0.44          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 15       | 0.44          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 16       | 0.44          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 18       | 0.44          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 9        | 0.44          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 18       | 0.44          |
| (1,2141) | 1:32:A:LYS:H     | 1:32:A:LYS:HG2   | 2        | 0.44          |
| (1,2002) | 1:79:B:TYR:H     | 1:111:B:VAL:HA   | 17       | 0.44          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 2        | 0.44          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG21 | 19       | 0.44          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG21 | 19       | 0.44          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG22  | 16       | 0.44          |
| (1,1446) | 1:25:B:LYS:HE3   | 1:25:B:LYS:HG2   | 3        | 0.44          |
| (1,1446) | 1:25:B:LYS:HE3   | 1:25:B:LYS:HG2   | 13       | 0.44          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 16       | 0.44          |
| (1,1436) | 1:38:B:VAL:HG23  | 1:28:B:ALA:HB3   | 10       | 0.44          |
| (1,1435) | 1:38:A:VAL:HG23  | 1:28:A:ALA:HB3   | 10       | 0.44          |
| (1,1204) | 1:37:B:MET:HE1   | 1:26:B:THR:HG23  | 2        | 0.44          |
| (1,924)  | 1:81:B:THR:HG22  | 1:111:B:VAL:HG11 | 10       | 0.44          |
| (1,923)  | 1:81:A:THR:HG22  | 1:111:A:VAL:HG11 | 10       | 0.44          |
| (1,912)  | 1:9:B:ARG:HB2    | 1:6:B:ILE:HG13   | 20       | 0.44          |
| (1,911)  | 1:9:A:ARG:HB2    | 1:6:A:ILE:HG13   | 20       | 0.44          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG23  | 14       | 0.44          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG23  | 14       | 0.44          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 20       | 0.44          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 12       | 0.44          |
| (1,554)  | 1:88:B:LYS:HG2   | 1:88:B:LYS:HE2   | 11       | 0.44          |
| (1,544)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD23  | 9        | 0.44          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 2        | 0.44          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 2        | 0.44          |
| (1,390)  | 1:102:B:ILE:HD13 | 1:38:B:VAL:HG12  | 9        | 0.44          |
| (1,390)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG11  | 16       | 0.44          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD12 | 8        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD12 | 11       | 0.44          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD13 | 14       | 0.44          |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD12 | 16       | 0.44          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD13 | 20       | 0.44          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD12 | 11       | 0.44          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD13 | 14       | 0.44          |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD12 | 16       | 0.44          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD13 | 20       | 0.44          |
| (1,292)  | 1:106:B:THR:H    | 1:106:B:THR:HG21 | 16       | 0.44          |
| (1,291)  | 1:106:A:THR:H    | 1:106:A:THR:HG21 | 16       | 0.44          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 20       | 0.44          |
| (1,158)  | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2   | 2        | 0.44          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2   | 18       | 0.44          |
| (1,3076) | 1:42:B:VAL:HG23  | 1:99:A:TRP:HE1   | 7        | 0.43          |
| (1,3052) | 1:21:B:TRP:HE1   | 1:31:A:ILE:HD13  | 5        | 0.43          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 9        | 0.43          |
| (1,2812) | 1:81:B:THR:H     | 1:79:B:TYR:HB2   | 16       | 0.43          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 16       | 0.43          |
| (1,2735) | 1:51:A:GLN:HE21  | 1:90:A:LEU:H     | 10       | 0.43          |
| (1,2604) | 1:107:B:ALA:H    | 1:82:B:THR:HA    | 11       | 0.43          |
| (1,2545) | 1:72:A:ASP:H     | 1:76:A:TRP:HE1   | 18       | 0.43          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 1        | 0.43          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 9        | 0.43          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 17       | 0.43          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 1        | 0.43          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 9        | 0.43          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 17       | 0.43          |
| (1,2142) | 1:32:B:LYS:H     | 1:32:B:LYS:HG2   | 2        | 0.43          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG22  | 16       | 0.43          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 5        | 0.43          |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 5        | 0.43          |
| (1,1446) | 1:25:B:LYS:HE3   | 1:25:B:LYS:HG2   | 7        | 0.43          |
| (1,1445) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HG2   | 7        | 0.43          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 19       | 0.43          |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG13  | 9        | 0.43          |
| (1,1388) | 1:20:B:VAL:HG12  | 1:19:B:SER:H     | 15       | 0.43          |
| (1,1387) | 1:20:A:VAL:HG12  | 1:19:A:SER:H     | 15       | 0.43          |
| (1,1383) | 1:18:A:VAL:HG23  | 1:59:A:ARG:HG2   | 1        | 0.43          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 8        | 0.43          |
| (1,1247) | 1:71:A:ILE:HG12  | 1:70:A:GLY:HA3   | 8        | 0.43          |
| (1,1203) | 1:37:A:MET:HE1   | 1:26:A:THR:HG23  | 2        | 0.43          |
| (1,1019) | 1:12:A:PHE:HB3   | 1:13:A:SER:HB2   | 2        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 20       | 0.43          |
| (1,596)  | 1:107:B:ALA:HB3  | 1:106:B:THR:HA   | 9        | 0.43          |
| (1,595)  | 1:107:A:ALA:HB3  | 1:106:A:THR:HA   | 9        | 0.43          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 14       | 0.43          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 12       | 0.43          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 14       | 0.43          |
| (1,543)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD23  | 9        | 0.43          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE1   | 15       | 0.43          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE1   | 15       | 0.43          |
| (1,392)  | 1:102:B:ILE:HD12 | 1:38:B:VAL:HG21  | 17       | 0.43          |
| (1,391)  | 1:102:A:ILE:HD12 | 1:38:A:VAL:HG21  | 17       | 0.43          |
| (1,389)  | 1:102:A:ILE:HD13 | 1:38:A:VAL:HG12  | 9        | 0.43          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD12 | 4        | 0.43          |
| (1,384)  | 1:104:B:ILE:HG22 | 1:104:B:ILE:HD12 | 7        | 0.43          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD12 | 4        | 0.43          |
| (1,383)  | 1:104:A:ILE:HG22 | 1:104:A:ILE:HD12 | 7        | 0.43          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 19       | 0.43          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 19       | 0.43          |
| (1,54)   | 1:42:B:VAL:HG22  | 1:99:B:TRP:HZ2   | 9        | 0.43          |
| (1,53)   | 1:42:A:VAL:HG22  | 1:99:A:TRP:HZ2   | 9        | 0.43          |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD13  | 6        | 0.42          |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD13  | 6        | 0.42          |
| (1,3084) | 1:13:B:SER:H     | 1:111:A:VAL:HA   | 17       | 0.42          |
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD1   | 15       | 0.42          |
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD2   | 16       | 0.42          |
| (1,3056) | 1:107:B:ALA:HB3  | 1:109:A:VAL:HG11 | 15       | 0.42          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 3        | 0.42          |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3   | 3        | 0.42          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 20       | 0.42          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 20       | 0.42          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 9        | 0.42          |
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 13       | 0.42          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 13       | 0.42          |
| (1,2546) | 1:72:B:ASP:H     | 1:76:B:TRP:HE1   | 18       | 0.42          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG22 | 10       | 0.42          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG22 | 10       | 0.42          |
| (1,2256) | 1:77:B:ASN:HD22  | 1:115:B:LYS:HG2  | 9        | 0.42          |
| (1,2255) | 1:77:A:ASN:HD22  | 1:115:A:LYS:HG2  | 9        | 0.42          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 10       | 0.42          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 10       | 0.42          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 2        | 0.42          |
| (1,1476) | 1:112:B:LEU:HD11 | 1:71:B:ILE:HA    | 8        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1475) | 1:112:A:LEU:HD11 | 1:71:A:ILE:HA    | 8        | 0.42          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 19       | 0.42          |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG13  | 9        | 0.42          |
| (1,1384) | 1:18:B:VAL:HG23  | 1:59:B:ARG:HG2   | 1        | 0.42          |
| (1,1020) | 1:12:B:PHE:HB3   | 1:13:B:SER:HB2   | 2        | 0.42          |
| (1,596)  | 1:107:B:ALA:HB3  | 1:106:B:THR:HA   | 4        | 0.42          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 20       | 0.42          |
| (1,595)  | 1:107:A:ALA:HB3  | 1:106:A:THR:HA   | 4        | 0.42          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 20       | 0.42          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE3   | 2        | 0.42          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE3   | 3        | 0.42          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE1   | 14       | 0.42          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE3   | 16       | 0.42          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE3   | 2        | 0.42          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE3   | 3        | 0.42          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE1   | 14       | 0.42          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE3   | 16       | 0.42          |
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 4        | 0.42          |
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 15       | 0.42          |
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 4        | 0.42          |
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 15       | 0.42          |
| (1,392)  | 1:102:B:ILE:HD11 | 1:38:B:VAL:HG22  | 7        | 0.42          |
| (1,391)  | 1:102:A:ILE:HD11 | 1:38:A:VAL:HG22  | 7        | 0.42          |
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB    | 12       | 0.42          |
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB    | 15       | 0.42          |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB    | 12       | 0.42          |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB    | 15       | 0.42          |
| (1,3075) | 1:42:A:VAL:HG21  | 1:99:B:TRP:HE1   | 3        | 0.41          |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD1   | 11       | 0.41          |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG11 | 1        | 0.41          |
| (1,3055) | 1:107:A:ALA:HB3  | 1:109:B:VAL:HG13 | 13       | 0.41          |
| (1,3055) | 1:107:A:ALA:HB3  | 1:109:B:VAL:HG11 | 15       | 0.41          |
| (1,3051) | 1:21:A:TRP:HE1   | 1:31:B:ILE:HD13  | 5        | 0.41          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG12  | 4        | 0.41          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG13  | 16       | 0.41          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG12  | 4        | 0.41          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG13  | 16       | 0.41          |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG22  | 15       | 0.41          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG22  | 15       | 0.41          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 19       | 0.41          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 19       | 0.41          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 5        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 7        | 0.41          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 5        | 0.41          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 7        | 0.41          |
| (1,2032) | 1:27:B:THR:H     | 1:38:B:VAL:HG21  | 10       | 0.41          |
| (1,2031) | 1:27:A:THR:H     | 1:38:A:VAL:HG21  | 10       | 0.41          |
| (1,2002) | 1:79:B:TYR:H     | 1:111:B:VAL:HA   | 6        | 0.41          |
| (1,2001) | 1:79:A:TYR:H     | 1:111:A:VAL:HA   | 6        | 0.41          |
| (1,1718) | 1:76:B:TRP:H     | 1:74:B:LYS:HD2   | 7        | 0.41          |
| (1,1384) | 1:18:B:VAL:HG22  | 1:59:B:ARG:HG2   | 11       | 0.41          |
| (1,1383) | 1:18:A:VAL:HG22  | 1:59:A:ARG:HG2   | 11       | 0.41          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 10       | 0.41          |
| (1,1247) | 1:71:A:ILE:HG12  | 1:70:A:GLY:HA3   | 10       | 0.41          |
| (1,1204) | 1:37:B:MET:HE1   | 1:26:B:THR:HG21  | 3        | 0.41          |
| (1,1204) | 1:37:B:MET:HE1   | 1:26:B:THR:HG22  | 11       | 0.41          |
| (1,1203) | 1:37:A:MET:HE1   | 1:26:A:THR:HG21  | 3        | 0.41          |
| (1,954)  | 1:18:B:VAL:HG23  | 1:59:B:ARG:HD2   | 4        | 0.41          |
| (1,953)  | 1:18:A:VAL:HG23  | 1:59:A:ARG:HD2   | 4        | 0.41          |
| (1,604)  | 1:104:B:ILE:HB   | 1:85:B:THR:HG23  | 2        | 0.41          |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG23  | 2        | 0.41          |
| (1,596)  | 1:107:B:ALA:HB2  | 1:106:B:THR:HA   | 11       | 0.41          |
| (1,554)  | 1:88:B:LYS:HG2   | 1:88:B:LYS:HE2   | 20       | 0.41          |
| (1,553)  | 1:88:A:LYS:HG2   | 1:88:A:LYS:HE2   | 20       | 0.41          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE1   | 1        | 0.41          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE2   | 5        | 0.41          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE1   | 9        | 0.41          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE1   | 1        | 0.41          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE2   | 5        | 0.41          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE2   | 7        | 0.41          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE1   | 9        | 0.41          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE1   | 19       | 0.41          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 12       | 0.41          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 19       | 0.41          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 12       | 0.41          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 10       | 0.41          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 10       | 0.41          |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD13 | 18       | 0.41          |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD13 | 17       | 0.41          |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD13 | 18       | 0.41          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 11       | 0.41          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 11       | 0.41          |
| (1,184)  | 1:94:B:GLY:HA2   | 1:95:B:LYS:HB2   | 2        | 0.41          |
| (1,183)  | 1:94:A:GLY:HA2   | 1:95:A:LYS:HB2   | 2        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,158)  | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2   | 16       | 0.41          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2   | 16       | 0.41          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB2   | 12       | 0.41          |
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB    | 14       | 0.41          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD21 | 18       | 0.4           |
| (1,3083) | 1:13:A:SER:H     | 1:111:B:VAL:HA   | 17       | 0.4           |
| (1,3076) | 1:42:B:VAL:HG21  | 1:99:A:TRP:HE1   | 3        | 0.4           |
| (1,3063) | 1:12:A:PHE:H     | 1:111:B:VAL:HG11 | 1        | 0.4           |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 14       | 0.4           |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3   | 14       | 0.4           |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 5        | 0.4           |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 7        | 0.4           |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 5        | 0.4           |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 7        | 0.4           |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG21  | 19       | 0.4           |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG21  | 19       | 0.4           |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG23 | 13       | 0.4           |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 8        | 0.4           |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 2        | 0.4           |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 11       | 0.4           |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 2        | 0.4           |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 11       | 0.4           |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 11       | 0.4           |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 11       | 0.4           |
| (1,2186) | 1:100:B:ARG:H    | 1:98:B:ALA:HB2   | 8        | 0.4           |
| (1,2185) | 1:100:A:ARG:H    | 1:98:A:ALA:HB2   | 8        | 0.4           |
| (1,1871) | 1:21:A:TRP:HE1   | 1:21:A:TRP:H     | 15       | 0.4           |
| (1,1717) | 1:76:A:TRP:H     | 1:74:A:LYS:HD2   | 7        | 0.4           |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG11  | 16       | 0.4           |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG11  | 16       | 0.4           |
| (1,1388) | 1:20:B:VAL:HG11  | 1:19:B:SER:H     | 17       | 0.4           |
| (1,1387) | 1:20:A:VAL:HG11  | 1:19:A:SER:H     | 17       | 0.4           |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22  | 7        | 0.4           |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22  | 7        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 1        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 2        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 3        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 4        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 5        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 6        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 7        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2   | 1:47:B:SER:HB3   | 8        | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 9        | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 10       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 11       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 12       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 13       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 14       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 15       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 16       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 17       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 18       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 19       | 0.4           |
| (1,1234) | 1:47:B:SER:HB2  | 1:47:B:SER:HB3  | 20       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 1        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 2        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 3        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 4        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 5        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 6        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 7        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 8        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 9        | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 10       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 11       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 12       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 13       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 14       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 15       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 16       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 17       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 18       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 19       | 0.4           |
| (1,1233) | 1:47:A:SER:HB2  | 1:47:A:SER:HB3  | 20       | 0.4           |
| (1,1203) | 1:37:A:MET:HE1  | 1:26:A:THR:HG22 | 11       | 0.4           |
| (1,1087) | 1:115:A:LYS:HG2 | 1:114:A:ARG:HA  | 8        | 0.4           |
| (1,960)  | 1:59:B:ARG:HD2  | 1:18:B:VAL:HB   | 13       | 0.4           |
| (1,595)  | 1:107:A:ALA:HB2 | 1:106:A:THR:HA  | 11       | 0.4           |
| (1,588)  | 1:115:B:LYS:HD2 | 1:115:B:LYS:HB3 | 1        | 0.4           |
| (1,587)  | 1:115:A:LYS:HD2 | 1:115:A:LYS:HB3 | 1        | 0.4           |
| (1,512)  | 1:37:B:MET:HG2  | 1:37:B:MET:HE2  | 7        | 0.4           |
| (1,512)  | 1:37:B:MET:HG2  | 1:37:B:MET:HE3  | 11       | 0.4           |
| (1,512)  | 1:37:B:MET:HG2  | 1:37:B:MET:HE1  | 19       | 0.4           |
| (1,511)  | 1:37:A:MET:HG2  | 1:37:A:MET:HE3  | 11       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 7        | 0.4           |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 7        | 0.4           |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 19       | 0.4           |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 8        | 0.4           |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD13 | 17       | 0.4           |
| (1,258)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HB2   | 6        | 0.4           |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB2   | 12       | 0.4           |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB    | 14       | 0.4           |
| (1,3)    | 1:111:A:VAL:HG22 | 1:112:A:LEU:HD22 | 18       | 0.4           |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD12  | 4        | 0.39          |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 8        | 0.39          |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 8        | 0.39          |
| (1,3089) | 1:112:A:LEU:HD22 | 1:14:B:VAL:HA    | 2        | 0.39          |
| (1,3086) | 1:112:B:LEU:HD12 | 1:14:A:VAL:HG22  | 6        | 0.39          |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD2   | 16       | 0.39          |
| (1,3059) | 1:71:A:ILE:HD12  | 1:14:B:VAL:HB    | 13       | 0.39          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 4        | 0.39          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 4        | 0.39          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 20       | 0.39          |
| (1,2862) | 1:73:B:SER:H     | 1:73:B:SER:HB2   | 13       | 0.39          |
| (1,2861) | 1:73:A:SER:H     | 1:73:A:SER:HB2   | 13       | 0.39          |
| (1,2850) | 1:72:B:ASP:H     | 1:73:B:SER:H     | 4        | 0.39          |
| (1,2849) | 1:72:A:ASP:H     | 1:73:A:SER:H     | 4        | 0.39          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 13       | 0.39          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 8        | 0.39          |
| (1,2150) | 1:77:B:ASN:H     | 1:112:B:LEU:HD23 | 7        | 0.39          |
| (1,2149) | 1:77:A:ASN:H     | 1:112:A:LEU:HD23 | 7        | 0.39          |
| (1,1872) | 1:21:B:TRP:HE1   | 1:21:B:TRP:H     | 15       | 0.39          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG22  | 5        | 0.39          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG22  | 5        | 0.39          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 7        | 0.39          |
| (1,1388) | 1:20:B:VAL:HG13  | 1:19:B:SER:H     | 2        | 0.39          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 2        | 0.39          |
| (1,1247) | 1:71:A:ILE:HG12  | 1:70:A:GLY:HA3   | 2        | 0.39          |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG23  | 16       | 0.39          |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG23  | 16       | 0.39          |
| (1,1088) | 1:115:B:LYS:HG2  | 1:114:B:ARG:HA   | 8        | 0.39          |
| (1,988)  | 1:27:B:THR:HG23  | 1:35:B:GLU:HG3   | 7        | 0.39          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 13       | 0.39          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB1  | 7        | 0.39          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG21  | 2        | 0.39          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG21  | 2        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,542)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD12  | 17       | 0.39          |
| (1,541)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD12  | 17       | 0.39          |
| (1,512)  | 1:37:B:MET:HG2   | 1:37:B:MET:HE3   | 4        | 0.39          |
| (1,511)  | 1:37:A:MET:HG2   | 1:37:A:MET:HE3   | 4        | 0.39          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 6        | 0.39          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 9        | 0.39          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 15       | 0.39          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 17       | 0.39          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 6        | 0.39          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 9        | 0.39          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 15       | 0.39          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 17       | 0.39          |
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 17       | 0.39          |
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 17       | 0.39          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 8        | 0.39          |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD12 | 2        | 0.39          |
| (1,384)  | 1:104:B:ILE:HG21 | 1:104:B:ILE:HD13 | 6        | 0.39          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD12 | 12       | 0.39          |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD12 | 2        | 0.39          |
| (1,383)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HD13 | 6        | 0.39          |
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD12 | 12       | 0.39          |
| (1,344)  | 1:48:B:VAL:HG13  | 1:41:B:GLU:HG2   | 2        | 0.39          |
| (1,257)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HB2   | 6        | 0.39          |
| (1,252)  | 1:112:B:LEU:HD22 | 1:71:B:ILE:HA    | 9        | 0.39          |
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB    | 9        | 0.39          |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB    | 9        | 0.39          |
| (1,4)    | 1:111:B:VAL:HG22 | 1:112:B:LEU:HD22 | 18       | 0.39          |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD12  | 4        | 0.38          |
| (1,3102) | 1:9:B:ARG:HB3    | 1:115:A:LYS:HA   | 5        | 0.38          |
| (1,3092) | 1:86:B:PHE:H     | 1:54:A:PHE:HD1   | 3        | 0.38          |
| (1,3080) | 1:11:B:GLU:HG2   | 1:111:A:VAL:HG21 | 12       | 0.38          |
| (1,3073) | 1:114:A:ARG:H    | 1:12:B:PHE:HD1   | 11       | 0.38          |
| (1,3058) | 1:70:B:GLY:HA2   | 1:76:A:TRP:HE1   | 12       | 0.38          |
| (1,3056) | 1:107:B:ALA:HB1  | 1:109:A:VAL:HG12 | 18       | 0.38          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 11       | 0.38          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 11       | 0.38          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD12  | 19       | 0.38          |
| (1,3040) | 1:35:B:GLU:H     | 1:34:B:LYS:HD3   | 10       | 0.38          |
| (1,3039) | 1:35:A:GLU:H     | 1:34:A:LYS:HD3   | 10       | 0.38          |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3   | 20       | 0.38          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11  | 20       | 0.38          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG11  | 20       | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 8        | 0.38          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 19       | 0.38          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG12 | 1        | 0.38          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG12 | 1        | 0.38          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 13       | 0.38          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 3        | 0.38          |
| (1,2196) | 1:55:B:GLU:H     | 1:22:B:VAL:HG11  | 5        | 0.38          |
| (1,2195) | 1:55:A:GLU:H     | 1:22:A:VAL:HG11  | 5        | 0.38          |
| (1,2152) | 1:77:B:ASN:H     | 1:115:B:LYS:HD2  | 2        | 0.38          |
| (1,2151) | 1:77:A:ASN:H     | 1:115:A:LYS:HD2  | 2        | 0.38          |
| (1,2151) | 1:77:A:ASN:H     | 1:115:A:LYS:HD2  | 13       | 0.38          |
| (1,1660) | 1:47:B:SER:H     | 1:47:B:SER:HB3   | 9        | 0.38          |
| (1,1659) | 1:47:A:SER:H     | 1:47:A:SER:HB3   | 9        | 0.38          |
| (1,1659) | 1:47:A:SER:H     | 1:47:A:SER:HB3   | 15       | 0.38          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 7        | 0.38          |
| (1,1387) | 1:20:A:VAL:HG13  | 1:19:A:SER:H     | 2        | 0.38          |
| (1,1376) | 1:74:B:LYS:HD2   | 1:74:B:LYS:HB2   | 7        | 0.38          |
| (1,1375) | 1:74:A:LYS:HD2   | 1:74:A:LYS:HB2   | 7        | 0.38          |
| (1,1216) | 1:22:B:VAL:HG13  | 1:20:B:VAL:HB    | 12       | 0.38          |
| (1,1215) | 1:22:A:VAL:HG13  | 1:20:A:VAL:HB    | 12       | 0.38          |
| (1,1204) | 1:37:B:MET:HE3   | 1:26:B:THR:HG23  | 5        | 0.38          |
| (1,1204) | 1:37:B:MET:HE3   | 1:26:B:THR:HG22  | 9        | 0.38          |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG23  | 19       | 0.38          |
| (1,1203) | 1:37:A:MET:HE3   | 1:26:A:THR:HG23  | 5        | 0.38          |
| (1,1203) | 1:37:A:MET:HE3   | 1:26:A:THR:HG22  | 9        | 0.38          |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG23  | 19       | 0.38          |
| (1,988)  | 1:27:B:THR:HG22  | 1:35:B:GLU:HG3   | 14       | 0.38          |
| (1,987)  | 1:27:A:THR:HG23  | 1:35:A:GLU:HG3   | 7        | 0.38          |
| (1,924)  | 1:81:B:THR:HG22  | 1:111:B:VAL:HG12 | 16       | 0.38          |
| (1,923)  | 1:81:A:THR:HG22  | 1:111:A:VAL:HG12 | 16       | 0.38          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB1  | 7        | 0.38          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 1        | 0.38          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 1        | 0.38          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 5        | 0.38          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 8        | 0.38          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3   | 11       | 0.38          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 1        | 0.38          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 5        | 0.38          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 8        | 0.38          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 11       | 0.38          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 14       | 0.38          |
| (1,384)  | 1:104:B:ILE:HG23 | 1:104:B:ILE:HD13 | 9        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,383)  | 1:104:A:ILE:HG23 | 1:104:A:ILE:HD13 | 9        | 0.38          |
| (1,343)  | 1:48:A:VAL:HG13  | 1:41:A:GLU:HG2   | 2        | 0.38          |
| (1,281)  | 1:37:A:MET:HA    | 1:37:A:MET:HE3   | 10       | 0.38          |
| (1,251)  | 1:112:A:LEU:HD22 | 1:71:A:ILE:HA    | 9        | 0.38          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 11       | 0.38          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 11       | 0.38          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H     | 13       | 0.37          |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 13       | 0.37          |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 13       | 0.37          |
| (1,3057) | 1:70:A:GLY:HA2   | 1:76:B:TRP:HE1   | 12       | 0.37          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 3        | 0.37          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 3        | 0.37          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 18       | 0.37          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 18       | 0.37          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 10       | 0.37          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 10       | 0.37          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 1        | 0.37          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 8        | 0.37          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 1        | 0.37          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG21  | 18       | 0.37          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG21  | 18       | 0.37          |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG23  | 7        | 0.37          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG23  | 7        | 0.37          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG22 | 9        | 0.37          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG22 | 9        | 0.37          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 1        | 0.37          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 1        | 0.37          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 19       | 0.37          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 6        | 0.37          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 6        | 0.37          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 2        | 0.37          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 2        | 0.37          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 6        | 0.37          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 13       | 0.37          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 3        | 0.37          |
| (1,2152) | 1:77:B:ASN:H     | 1:115:B:LYS:HD2  | 13       | 0.37          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 11       | 0.37          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 11       | 0.37          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 16       | 0.37          |
| (1,1660) | 1:47:B:SER:H     | 1:47:B:SER:HB3   | 15       | 0.37          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG22  | 1        | 0.37          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG23  | 18       | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1542) | 1:54:B:PHE:HB2  | 1:55:B:GLU:HG3  | 10       | 0.37          |
| (1,1541) | 1:54:A:PHE:HB2  | 1:55:A:GLU:HG3  | 10       | 0.37          |
| (1,1388) | 1:20:B:VAL:HG13 | 1:19:B:SER:H    | 7        | 0.37          |
| (1,1387) | 1:20:A:VAL:HG13 | 1:19:A:SER:H    | 7        | 0.37          |
| (1,1314) | 1:70:B:GLY:H    | 1:64:B:VAL:HG13 | 1        | 0.37          |
| (1,1313) | 1:70:A:GLY:H    | 1:64:A:VAL:HG13 | 1        | 0.37          |
| (1,1216) | 1:22:B:VAL:HG11 | 1:20:B:VAL:HB   | 10       | 0.37          |
| (1,987)  | 1:27:A:THR:HG22 | 1:35:A:GLU:HG3  | 14       | 0.37          |
| (1,588)  | 1:115:B:LYS:HD2 | 1:115:B:LYS:HB3 | 11       | 0.37          |
| (1,587)  | 1:115:A:LYS:HD2 | 1:115:A:LYS:HB3 | 11       | 0.37          |
| (1,584)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HD2 | 1        | 0.37          |
| (1,480)  | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG3  | 4        | 0.37          |
| (1,480)  | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG3  | 14       | 0.37          |
| (1,480)  | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG3  | 20       | 0.37          |
| (1,479)  | 1:32:A:LYS:HD2  | 1:32:A:LYS:HG3  | 20       | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 1        | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 3        | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 5        | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 8        | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 9        | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 10       | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 12       | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 14       | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 16       | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 18       | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 19       | 0.37          |
| (1,360)  | 1:41:B:GLU:HG2  | 1:41:B:GLU:HB2  | 20       | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 1        | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 3        | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 5        | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 8        | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 9        | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 10       | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 12       | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 14       | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 16       | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 18       | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 19       | 0.37          |
| (1,359)  | 1:41:A:GLU:HG2  | 1:41:A:GLU:HB2  | 20       | 0.37          |
| (1,308)  | 1:71:B:ILE:HG21 | 1:76:B:TRP:HB3  | 17       | 0.37          |
| (1,307)  | 1:71:A:ILE:HG21 | 1:76:A:TRP:HB3  | 17       | 0.37          |
| (1,282)  | 1:37:B:MET:HA   | 1:37:B:MET:HE3  | 10       | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,258)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HB2   | 19       | 0.37          |
| (1,257)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HB2   | 19       | 0.37          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 15       | 0.37          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 15       | 0.37          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 13       | 0.36          |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD13  | 19       | 0.36          |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD13  | 19       | 0.36          |
| (1,3101) | 1:9:A:ARG:HB3    | 1:115:B:LYS:HA   | 5        | 0.36          |
| (1,3091) | 1:86:A:PHE:H     | 1:54:B:PHE:HD1   | 3        | 0.36          |
| (1,3091) | 1:86:A:PHE:H     | 1:54:B:PHE:HD2   | 4        | 0.36          |
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG21 | 12       | 0.36          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 8        | 0.36          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 8        | 0.36          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG11  | 6        | 0.36          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG11  | 6        | 0.36          |
| (1,2998) | 1:77:B:ASN:HD22  | 1:115:B:LYS:H    | 18       | 0.36          |
| (1,2997) | 1:77:A:ASN:HD22  | 1:115:A:LYS:H    | 18       | 0.36          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 2        | 0.36          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 2        | 0.36          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 15       | 0.36          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 15       | 0.36          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 2        | 0.36          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG21  | 7        | 0.36          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 11       | 0.36          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 2        | 0.36          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 7        | 0.36          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 11       | 0.36          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 7        | 0.36          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 6        | 0.36          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 7        | 0.36          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 8        | 0.36          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 16       | 0.36          |
| (1,1872) | 1:21:B:TRP:HE1   | 1:21:B:TRP:H     | 14       | 0.36          |
| (1,1871) | 1:21:A:TRP:HE1   | 1:21:A:TRP:H     | 14       | 0.36          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG23  | 7        | 0.36          |
| (1,1660) | 1:47:B:SER:H     | 1:47:B:SER:HB3   | 11       | 0.36          |
| (1,1660) | 1:47:B:SER:H     | 1:47:B:SER:HB3   | 18       | 0.36          |
| (1,1660) | 1:47:B:SER:H     | 1:47:B:SER:HB3   | 20       | 0.36          |
| (1,1659) | 1:47:A:SER:H     | 1:47:A:SER:HB3   | 18       | 0.36          |
| (1,1659) | 1:47:A:SER:H     | 1:47:A:SER:HB3   | 20       | 0.36          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG12  | 2        | 0.36          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG11  | 3        | 0.36          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1649) | 1:47:A:SER:H     | 1:48:A:VAL:HG12 | 2        | 0.36          |
| (1,1649) | 1:47:A:SER:H     | 1:48:A:VAL:HG11 | 3        | 0.36          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG22 | 1        | 0.36          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG23 | 18       | 0.36          |
| (1,1482) | 1:112:B:LEU:HD11 | 1:76:B:TRP:HB2  | 11       | 0.36          |
| (1,1481) | 1:112:A:LEU:HD11 | 1:76:A:TRP:HB2  | 11       | 0.36          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG12 | 5        | 0.36          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG12 | 5        | 0.36          |
| (1,1376) | 1:74:B:LYS:HD2   | 1:74:B:LYS:HB2  | 1        | 0.36          |
| (1,1375) | 1:74:A:LYS:HD2   | 1:74:A:LYS:HB2  | 1        | 0.36          |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22 | 8        | 0.36          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22 | 8        | 0.36          |
| (1,1216) | 1:22:B:VAL:HG12  | 1:20:B:VAL:HB   | 14       | 0.36          |
| (1,1215) | 1:22:A:VAL:HG11  | 1:20:A:VAL:HB   | 10       | 0.36          |
| (1,1215) | 1:22:A:VAL:HG12  | 1:20:A:VAL:HB   | 14       | 0.36          |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG21 | 1        | 0.36          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB   | 10       | 0.36          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB   | 10       | 0.36          |
| (1,954)  | 1:18:B:VAL:HG22  | 1:59:B:ARG:HD2  | 15       | 0.36          |
| (1,953)  | 1:18:A:VAL:HG22  | 1:59:A:ARG:HD2  | 15       | 0.36          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB3 | 17       | 0.36          |
| (1,766)  | 1:102:B:ILE:HG12 | 1:38:B:VAL:HG22 | 18       | 0.36          |
| (1,765)  | 1:102:A:ILE:HG12 | 1:38:A:VAL:HG22 | 18       | 0.36          |
| (1,596)  | 1:107:B:ALA:HB2  | 1:106:B:THR:HA  | 14       | 0.36          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2  | 3        | 0.36          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2  | 6        | 0.36          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2  | 13       | 0.36          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2  | 17       | 0.36          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2  | 18       | 0.36          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2  | 2        | 0.36          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2  | 3        | 0.36          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2  | 6        | 0.36          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2  | 13       | 0.36          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2  | 17       | 0.36          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2  | 18       | 0.36          |
| (1,480)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG3  | 16       | 0.36          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3  | 4        | 0.36          |
| (1,360)  | 1:41:B:GLU:HG2   | 1:41:B:GLU:HB2  | 2        | 0.36          |
| (1,359)  | 1:41:A:GLU:HG2   | 1:41:A:GLU:HB2  | 2        | 0.36          |
| (1,250)  | 1:112:B:LEU:HD21 | 1:76:B:TRP:HD1  | 4        | 0.36          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1  | 15       | 0.36          |
| (1,249)  | 1:112:A:LEU:HD21 | 1:76:A:TRP:HD1  | 4        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 15       | 0.36          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 10       | 0.36          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB2   | 13       | 0.36          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 20       | 0.36          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 10       | 0.36          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB2   | 13       | 0.36          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 20       | 0.36          |
| (1,3100) | 1:9:B:ARG:HB2    | 1:117:A:VAL:HG22 | 9        | 0.35          |
| (1,3074) | 1:114:B:ARG:H    | 1:12:A:PHE:HD1   | 15       | 0.35          |
| (1,3056) | 1:107:B:ALA:HB3  | 1:109:A:VAL:HG13 | 13       | 0.35          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG13  | 14       | 0.35          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 12       | 0.35          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 12       | 0.35          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG11  | 3        | 0.35          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG13  | 5        | 0.35          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG11  | 3        | 0.35          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG13  | 5        | 0.35          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 15       | 0.35          |
| (1,2811) | 1:81:A:THR:H     | 1:79:A:TYR:HB2   | 10       | 0.35          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG22  | 8        | 0.35          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG21  | 13       | 0.35          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG21  | 13       | 0.35          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG22  | 14       | 0.35          |
| (1,2330) | 1:75:B:HIS:H     | 1:74:B:LYS:H     | 14       | 0.35          |
| (1,2329) | 1:75:A:HIS:H     | 1:74:A:LYS:H     | 14       | 0.35          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG13 | 13       | 0.35          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 5        | 0.35          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2  | 8        | 0.35          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 8        | 0.35          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 8        | 0.35          |
| (1,1872) | 1:21:B:TRP:HE1   | 1:21:B:TRP:H     | 10       | 0.35          |
| (1,1762) | 1:20:B:VAL:H     | 1:55:B:GLU:H     | 9        | 0.35          |
| (1,1761) | 1:20:A:VAL:H     | 1:55:A:GLU:H     | 9        | 0.35          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG23  | 7        | 0.35          |
| (1,1660) | 1:47:B:SER:H     | 1:47:B:SER:HB3   | 13       | 0.35          |
| (1,1659) | 1:47:A:SER:H     | 1:47:A:SER:HB3   | 11       | 0.35          |
| (1,1659) | 1:47:A:SER:H     | 1:47:A:SER:HB3   | 13       | 0.35          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 17       | 0.35          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 17       | 0.35          |
| (1,1297) | 1:36:A:VAL:HG21  | 1:91:A:THR:H     | 1        | 0.35          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 6        | 0.35          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 12       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1247) | 1:71:A:ILE:HG12  | 1:70:A:GLY:HA3   | 12       | 0.35          |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG21  | 1        | 0.35          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 7        | 0.35          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 8        | 0.35          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 8        | 0.35          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB3  | 17       | 0.35          |
| (1,809)  | 1:118:A:ARG:HB2  | 1:118:A:ARG:HG2  | 8        | 0.35          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 18       | 0.35          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 18       | 0.35          |
| (1,595)  | 1:107:A:ALA:HB2  | 1:106:A:THR:HA   | 14       | 0.35          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2   | 1        | 0.35          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2   | 2        | 0.35          |
| (1,566)  | 1:57:B:LYS:HD2   | 1:57:B:LYS:HG2   | 12       | 0.35          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2   | 1        | 0.35          |
| (1,565)  | 1:57:A:LYS:HD2   | 1:57:A:LYS:HG2   | 12       | 0.35          |
| (1,479)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG3   | 16       | 0.35          |
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 9        | 0.35          |
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 9        | 0.35          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG23  | 7        | 0.35          |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG23  | 7        | 0.35          |
| (1,360)  | 1:41:B:GLU:HG2   | 1:41:B:GLU:HB2   | 7        | 0.35          |
| (1,360)  | 1:41:B:GLU:HG2   | 1:41:B:GLU:HB2   | 17       | 0.35          |
| (1,359)  | 1:41:A:GLU:HG2   | 1:41:A:GLU:HB2   | 7        | 0.35          |
| (1,359)  | 1:41:A:GLU:HG2   | 1:41:A:GLU:HB2   | 17       | 0.35          |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE1   | 8        | 0.35          |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE2   | 20       | 0.35          |
| (1,281)  | 1:37:A:MET:HA    | 1:37:A:MET:HE2   | 20       | 0.35          |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 8        | 0.35          |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 8        | 0.35          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 3        | 0.35          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 3        | 0.35          |
| (1,158)  | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2   | 3        | 0.35          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2   | 3        | 0.35          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 3        | 0.35          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 3        | 0.35          |
| (1,4)    | 1:111:B:VAL:HG23 | 1:112:B:LEU:HD22 | 11       | 0.35          |
| (1,3099) | 1:9:A:ARG:HB2    | 1:117:B:VAL:HG22 | 9        | 0.34          |
| (1,3094) | 1:86:B:PHE:H     | 1:54:A:PHE:HE2   | 11       | 0.34          |
| (1,3093) | 1:86:A:PHE:H     | 1:54:B:PHE:HE2   | 11       | 0.34          |
| (1,3087) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HA    | 6        | 0.34          |
| (1,3076) | 1:42:B:VAL:HG22  | 1:99:A:TRP:HE1   | 16       | 0.34          |
| (1,3075) | 1:42:A:VAL:HG22  | 1:99:B:TRP:HE1   | 16       | 0.34          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3066) | 1:11:B:GLU:HA   | 1:111:A:VAL:HG11 | 5        | 0.34          |
| (1,3065) | 1:11:A:GLU:HA   | 1:111:B:VAL:HG11 | 5        | 0.34          |
| (1,3056) | 1:107:B:ALA:HB2 | 1:109:A:VAL:HG13 | 12       | 0.34          |
| (1,3050) | 1:21:B:TRP:HH2  | 1:31:A:ILE:HD13  | 4        | 0.34          |
| (1,3027) | 1:35:A:GLU:H    | 1:36:A:VAL:HG11  | 10       | 0.34          |
| (1,2988) | 1:103:B:ARG:H   | 1:102:B:ILE:HG13 | 15       | 0.34          |
| (1,2906) | 1:22:B:VAL:H    | 1:53:B:PHE:HB3   | 11       | 0.34          |
| (1,2905) | 1:22:A:VAL:H    | 1:53:A:PHE:HB3   | 11       | 0.34          |
| (1,2812) | 1:81:B:THR:H    | 1:79:B:TYR:HB2   | 10       | 0.34          |
| (1,2386) | 1:29:B:THR:H    | 1:29:B:THR:HG22  | 14       | 0.34          |
| (1,2386) | 1:29:B:THR:H    | 1:29:B:THR:HG21  | 15       | 0.34          |
| (1,2386) | 1:29:B:THR:H    | 1:29:B:THR:HG22  | 16       | 0.34          |
| (1,2385) | 1:29:A:THR:H    | 1:29:A:THR:HG22  | 8        | 0.34          |
| (1,2385) | 1:29:A:THR:H    | 1:29:A:THR:HG21  | 15       | 0.34          |
| (1,2385) | 1:29:A:THR:H    | 1:29:A:THR:HG22  | 16       | 0.34          |
| (1,2231) | 1:118:A:ARG:H   | 1:117:A:VAL:HG13 | 13       | 0.34          |
| (1,2228) | 1:118:B:ARG:H   | 1:117:B:VAL:HA   | 4        | 0.34          |
| (1,2227) | 1:118:A:ARG:H   | 1:117:A:VAL:HA   | 4        | 0.34          |
| (1,2227) | 1:118:A:ARG:H   | 1:117:A:VAL:HA   | 14       | 0.34          |
| (1,2226) | 1:118:B:ARG:H   | 1:118:B:ARG:HA   | 5        | 0.34          |
| (1,2222) | 1:118:B:ARG:H   | 1:117:B:VAL:HB   | 17       | 0.34          |
| (1,2221) | 1:118:A:ARG:H   | 1:117:A:VAL:HB   | 17       | 0.34          |
| (1,2032) | 1:27:B:THR:H    | 1:38:B:VAL:HG23  | 3        | 0.34          |
| (1,2031) | 1:27:A:THR:H    | 1:38:A:VAL:HG23  | 3        | 0.34          |
| (1,1880) | 1:21:B:TRP:H    | 1:20:B:VAL:HG21  | 10       | 0.34          |
| (1,1879) | 1:21:A:TRP:H    | 1:20:A:VAL:HG21  | 10       | 0.34          |
| (1,1871) | 1:21:A:TRP:HE1  | 1:21:A:TRP:H     | 10       | 0.34          |
| (1,1314) | 1:70:B:GLY:H    | 1:64:B:VAL:HG12  | 2        | 0.34          |
| (1,1313) | 1:70:A:GLY:H    | 1:64:A:VAL:HG12  | 2        | 0.34          |
| (1,1298) | 1:36:B:VAL:HG21 | 1:91:B:THR:H     | 1        | 0.34          |
| (1,1247) | 1:71:A:ILE:HG12 | 1:70:A:GLY:HA3   | 6        | 0.34          |
| (1,1215) | 1:22:A:VAL:HG13 | 1:20:A:VAL:HB    | 11       | 0.34          |
| (1,1204) | 1:37:B:MET:HE3  | 1:26:B:THR:HG22  | 7        | 0.34          |
| (1,1188) | 1:31:B:ILE:HD12 | 1:101:B:PHE:HB2  | 10       | 0.34          |
| (1,1187) | 1:31:A:ILE:HD12 | 1:101:A:PHE:HB2  | 10       | 0.34          |
| (1,1171) | 1:39:A:LEU:HD22 | 1:92:A:MET:HG2   | 14       | 0.34          |
| (1,1162) | 1:95:B:LYS:H    | 1:95:B:LYS:HE3   | 16       | 0.34          |
| (1,1161) | 1:95:A:LYS:H    | 1:95:A:LYS:HE3   | 16       | 0.34          |
| (1,959)  | 1:59:A:ARG:HD2  | 1:18:A:VAL:HB    | 7        | 0.34          |
| (1,874)  | 1:39:B:LEU:HD12 | 1:91:B:THR:HA    | 13       | 0.34          |
| (1,873)  | 1:39:A:LEU:HD12 | 1:91:A:THR:HA    | 13       | 0.34          |
| (1,810)  | 1:118:B:ARG:HB2 | 1:118:B:ARG:HG2  | 8        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 6        | 0.34          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 6        | 0.34          |
| (1,542)  | 1:92:B:MET:HE1   | 1:39:B:LEU:HD12  | 6        | 0.34          |
| (1,454)  | 1:95:B:LYS:HB2   | 1:95:B:LYS:HD2   | 1        | 0.34          |
| (1,453)  | 1:95:A:LYS:HB2   | 1:95:A:LYS:HD2   | 1        | 0.34          |
| (1,416)  | 1:39:B:LEU:H     | 1:38:B:VAL:HG13  | 13       | 0.34          |
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG13  | 13       | 0.34          |
| (1,281)  | 1:37:A:MET:HA    | 1:37:A:MET:HE1   | 8        | 0.34          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 16       | 0.34          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 16       | 0.34          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 5        | 0.34          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB3   | 16       | 0.34          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 5        | 0.34          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 6        | 0.34          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB3   | 16       | 0.34          |
| (1,3)    | 1:111:A:VAL:HG23 | 1:112:A:LEU:HD22 | 11       | 0.34          |
| (1,3092) | 1:86:B:PHE:H     | 1:54:A:PHE:HD2   | 4        | 0.33          |
| (1,3089) | 1:112:A:LEU:HD22 | 1:14:B:VAL:HA    | 20       | 0.33          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11  | 10       | 0.33          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG11  | 17       | 0.33          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG13  | 14       | 0.33          |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 11       | 0.33          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 7        | 0.33          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 7        | 0.33          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG21  | 3        | 0.33          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG22  | 4        | 0.33          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG22  | 9        | 0.33          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG22  | 10       | 0.33          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG21  | 12       | 0.33          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 17       | 0.33          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 18       | 0.33          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG21  | 3        | 0.33          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG22  | 4        | 0.33          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG22  | 9        | 0.33          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG22  | 10       | 0.33          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 17       | 0.33          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 18       | 0.33          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 14       | 0.33          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 17       | 0.33          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 20       | 0.33          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 20       | 0.33          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 5        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 5        | 0.33          |
| (1,1996) | 1:67:B:GLY:H     | 1:64:B:VAL:HB    | 15       | 0.33          |
| (1,1995) | 1:67:A:GLY:H     | 1:64:A:VAL:HB    | 15       | 0.33          |
| (1,1880) | 1:21:B:TRP:H     | 1:20:B:VAL:HG22  | 17       | 0.33          |
| (1,1879) | 1:21:A:TRP:H     | 1:20:A:VAL:HG22  | 17       | 0.33          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG12  | 4        | 0.33          |
| (1,1476) | 1:112:B:LEU:HD13 | 1:71:B:ILE:HA    | 2        | 0.33          |
| (1,1475) | 1:112:A:LEU:HD13 | 1:71:A:ILE:HA    | 2        | 0.33          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 3        | 0.33          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 3        | 0.33          |
| (1,1216) | 1:22:B:VAL:HG13  | 1:20:B:VAL:HB    | 11       | 0.33          |
| (1,1203) | 1:37:A:MET:HE3   | 1:26:A:THR:HG22  | 7        | 0.33          |
| (1,1172) | 1:39:B:LEU:HD22  | 1:92:B:MET:HG2   | 14       | 0.33          |
| (1,988)  | 1:27:B:THR:HG23  | 1:35:B:GLU:HG3   | 18       | 0.33          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 15       | 0.33          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 15       | 0.33          |
| (1,541)  | 1:92:A:MET:HE1   | 1:39:A:LEU:HD12  | 6        | 0.33          |
| (1,440)  | 1:88:B:LYS:HA    | 1:88:B:LYS:HE2   | 13       | 0.33          |
| (1,439)  | 1:88:A:LYS:HA    | 1:88:A:LYS:HE2   | 13       | 0.33          |
| (1,424)  | 1:87:B:VAL:HG13  | 1:53:B:PHE:HD1   | 19       | 0.33          |
| (1,423)  | 1:87:A:VAL:HG13  | 1:53:A:PHE:HD1   | 19       | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG13 | 1        | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 5        | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 6        | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG13 | 7        | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 9        | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 12       | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG13 | 13       | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG12 | 16       | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG12 | 18       | 0.33          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 19       | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 1        | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 5        | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 6        | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG13 | 7        | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 9        | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 12       | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG13 | 13       | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 16       | 0.33          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 18       | 0.33          |
| (1,288)  | 1:106:B:THR:HG22 | 1:85:B:THR:HG21  | 15       | 0.33          |
| (1,287)  | 1:106:A:THR:HG22 | 1:85:A:THR:HG21  | 15       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,158)  | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2   | 20       | 0.33          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2   | 20       | 0.33          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 6        | 0.33          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 11       | 0.33          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 11       | 0.33          |
| (1,72)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG2   | 3        | 0.33          |
| (1,72)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG2   | 4        | 0.33          |
| (1,71)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG2   | 3        | 0.33          |
| (1,71)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG2   | 4        | 0.33          |
| (1,3)    | 1:111:A:VAL:HG22 | 1:112:A:LEU:HD22 | 10       | 0.33          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H     | 9        | 0.32          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 9        | 0.32          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD23 | 5        | 0.32          |
| (1,3055) | 1:107:A:ALA:HB1  | 1:109:B:VAL:HG12 | 18       | 0.32          |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD12  | 19       | 0.32          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD13  | 4        | 0.32          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG11  | 17       | 0.32          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 4        | 0.32          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 9        | 0.32          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 4        | 0.32          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 9        | 0.32          |
| (1,2976) | 1:103:B:ARG:H    | 1:103:B:ARG:HG2  | 11       | 0.32          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 14       | 0.32          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 14       | 0.32          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG21  | 12       | 0.32          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 17       | 0.32          |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 4        | 0.32          |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 4        | 0.32          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 14       | 0.32          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 14       | 0.32          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 4        | 0.32          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 4        | 0.32          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG22  | 14       | 0.32          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG21  | 1        | 0.32          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG22  | 14       | 0.32          |
| (1,1649) | 1:47:A:SER:H     | 1:48:A:VAL:HG12  | 4        | 0.32          |
| (1,1606) | 1:24:B:ASP:H     | 1:25:B:LYS:H     | 17       | 0.32          |
| (1,1605) | 1:24:A:ASP:H     | 1:25:A:LYS:H     | 17       | 0.32          |
| (1,1442) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HD1   | 4        | 0.32          |
| (1,1441) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HD1   | 4        | 0.32          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG13  | 2        | 0.32          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG13  | 2        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG23  | 12       | 0.32          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG22  | 14       | 0.32          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG23  | 12       | 0.32          |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG22  | 14       | 0.32          |
| (1,1347) | 1:87:A:VAL:HG13  | 1:104:A:ILE:HD12 | 6        | 0.32          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG11  | 2        | 0.32          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG11  | 2        | 0.32          |
| (1,1204) | 1:37:B:MET:HE1   | 1:26:B:THR:HG21  | 4        | 0.32          |
| (1,1203) | 1:37:A:MET:HE1   | 1:26:A:THR:HG21  | 4        | 0.32          |
| (1,1172) | 1:39:B:LEU:HD23  | 1:92:B:MET:HG2   | 7        | 0.32          |
| (1,987)  | 1:27:A:THR:HG23  | 1:35:A:GLU:HG3   | 18       | 0.32          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 14       | 0.32          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 14       | 0.32          |
| (1,424)  | 1:87:B:VAL:HG11  | 1:53:B:PHE:HD1   | 16       | 0.32          |
| (1,423)  | 1:87:A:VAL:HG11  | 1:53:A:PHE:HD1   | 16       | 0.32          |
| (1,416)  | 1:39:B:LEU:H     | 1:38:B:VAL:HG11  | 9        | 0.32          |
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG11  | 7        | 0.32          |
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG11  | 9        | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 2        | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG13 | 3        | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG12 | 8        | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 10       | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG13 | 11       | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG12 | 14       | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 17       | 0.32          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG12 | 20       | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 2        | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG13 | 3        | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 8        | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 10       | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG13 | 11       | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 14       | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 17       | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 19       | 0.32          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG12 | 20       | 0.32          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 2        | 0.32          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 10       | 0.32          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 13       | 0.32          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 15       | 0.32          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 16       | 0.32          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 18       | 0.32          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 19       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 2        | 0.32          |
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 10       | 0.32          |
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 13       | 0.32          |
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 15       | 0.32          |
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 16       | 0.32          |
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 18       | 0.32          |
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 19       | 0.32          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB2   | 9        | 0.32          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB2   | 9        | 0.32          |
| (1,72)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG2   | 13       | 0.32          |
| (1,72)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG2   | 18       | 0.32          |
| (1,71)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG2   | 13       | 0.32          |
| (1,71)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG2   | 18       | 0.32          |
| (1,48)   | 1:42:B:VAL:HG23  | 1:44:B:ILE:HB    | 16       | 0.32          |
| (1,47)   | 1:42:A:VAL:HG23  | 1:44:A:ILE:HB    | 16       | 0.32          |
| (1,4)    | 1:111:B:VAL:HG22 | 1:112:B:LEU:HD22 | 10       | 0.32          |
| (3,16)   | 1:28:B:ALA:H     | 1:103:B:ARG:H    | 6        | 0.31          |
| (3,15)   | 1:28:A:ALA:H     | 1:103:A:ARG:H    | 6        | 0.31          |
| (1,3095) | 1:69:A:ARG:HA    | 1:112:B:LEU:HD23 | 5        | 0.31          |
| (1,3090) | 1:112:B:LEU:HD22 | 1:14:A:VAL:HA    | 20       | 0.31          |
| (1,3088) | 1:112:B:LEU:HD13 | 1:14:A:VAL:HA    | 13       | 0.31          |
| (1,3055) | 1:107:A:ALA:HB2  | 1:109:B:VAL:HG13 | 12       | 0.31          |
| (1,3028) | 1:35:B:GLU:H     | 1:36:B:VAL:HG13  | 6        | 0.31          |
| (1,3027) | 1:35:A:GLU:H     | 1:36:A:VAL:HG13  | 6        | 0.31          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 13       | 0.31          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 13       | 0.31          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 20       | 0.31          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 20       | 0.31          |
| (1,2720) | 1:84:B:HIS:H     | 1:83:B:THR:HB    | 9        | 0.31          |
| (1,2719) | 1:84:A:HIS:H     | 1:83:A:THR:HB    | 9        | 0.31          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG21  | 15       | 0.31          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG21  | 15       | 0.31          |
| (1,2548) | 1:76:B:TRP:HE1   | 1:71:B:ILE:HG21  | 10       | 0.31          |
| (1,2547) | 1:76:A:TRP:HE1   | 1:71:A:ILE:HG21  | 10       | 0.31          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG21  | 1        | 0.31          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 5        | 0.31          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG21  | 1        | 0.31          |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 5        | 0.31          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 3        | 0.31          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 4        | 0.31          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 12       | 0.31          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 12       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG21  | 1        | 0.31          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG22 | 9        | 0.31          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG22 | 9        | 0.31          |
| (1,1577) | 1:45:A:ASN:HD21  | 1:44:A:ILE:HA    | 5        | 0.31          |
| (1,1556) | 1:49:B:PHE:HA    | 1:48:B:VAL:HB    | 11       | 0.31          |
| (1,1555) | 1:49:A:PHE:HA    | 1:48:A:VAL:HB    | 11       | 0.31          |
| (1,1492) | 1:71:B:ILE:HD11  | 1:14:B:VAL:HG22  | 10       | 0.31          |
| (1,1491) | 1:71:A:ILE:HD11  | 1:14:A:VAL:HG22  | 10       | 0.31          |
| (1,1388) | 1:20:B:VAL:HG12  | 1:19:B:SER:H     | 4        | 0.31          |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22  | 10       | 0.31          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22  | 4        | 0.31          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22  | 10       | 0.31          |
| (1,1348) | 1:87:B:VAL:HG13  | 1:104:B:ILE:HD12 | 6        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 1        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG11  | 3        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 4        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 5        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 6        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG11  | 7        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 8        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 9        | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 10       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 11       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG11  | 12       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 13       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 14       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 15       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG11  | 16       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 18       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG13  | 19       | 0.31          |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 20       | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 1        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG11  | 3        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 4        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 5        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 6        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG11  | 7        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 8        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 9        | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 11       | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 13       | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 14       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 15       | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG11  | 16       | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 18       | 0.31          |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 20       | 0.31          |
| (1,1171) | 1:39:A:LEU:HD23  | 1:92:A:MET:HG2   | 7        | 0.31          |
| (1,912)  | 1:9:B:ARG:HB2    | 1:6:B:ILE:HG13   | 10       | 0.31          |
| (1,911)  | 1:9:A:ARG:HB2    | 1:6:A:ILE:HG13   | 10       | 0.31          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 4        | 0.31          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 4        | 0.31          |
| (1,656)  | 1:42:B:VAL:HG13  | 1:99:B:TRP:HZ3   | 20       | 0.31          |
| (1,655)  | 1:42:A:VAL:HG13  | 1:99:A:TRP:HZ3   | 20       | 0.31          |
| (1,542)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD11  | 2        | 0.31          |
| (1,541)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD11  | 2        | 0.31          |
| (1,416)  | 1:39:B:LEU:H     | 1:38:B:VAL:HG11  | 7        | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 3        | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 4        | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 7        | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 8        | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 10       | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 14       | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 15       | 0.31          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 16       | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 3        | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 4        | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 7        | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 8        | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD12 | 9        | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 10       | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 14       | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 15       | 0.31          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 16       | 0.31          |
| (1,364)  | 1:117:B:VAL:HB   | 1:117:B:VAL:HG13 | 15       | 0.31          |
| (1,363)  | 1:117:A:VAL:HB   | 1:117:A:VAL:HG13 | 15       | 0.31          |
| (1,298)  | 1:118:B:ARG:HB3  | 1:118:B:ARG:HG2  | 17       | 0.31          |
| (1,297)  | 1:118:A:ARG:HB3  | 1:118:A:ARG:HG2  | 17       | 0.31          |
| (1,272)  | 1:14:B:VAL:HG11  | 1:15:B:CYS:HB2   | 9        | 0.31          |
| (1,271)  | 1:14:A:VAL:HG11  | 1:15:A:CYS:HB2   | 9        | 0.31          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 2        | 0.31          |
| (1,157)  | 1:40:A:GLY:HA2   | 1:41:A:GLU:HG2   | 8        | 0.31          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 15       | 0.31          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB3   | 7        | 0.31          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 17       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 19       | 0.31          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB3   | 7        | 0.31          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB2   | 15       | 0.31          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 17       | 0.31          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 19       | 0.31          |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG21 | 6        | 0.31          |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG21 | 6        | 0.31          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H     | 10       | 0.3           |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 10       | 0.3           |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 20       | 0.3           |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 20       | 0.3           |
| (1,2543) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD21 | 2        | 0.3           |
| (1,2385) | 1:29:A:THR:H     | 1:29:A:THR:HG23  | 20       | 0.3           |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 3        | 0.3           |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 7        | 0.3           |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 7        | 0.3           |
| (1,2226) | 1:118:B:ARG:H    | 1:118:B:ARG:HA   | 3        | 0.3           |
| (1,2225) | 1:118:A:ARG:H    | 1:118:A:ARG:HA   | 3        | 0.3           |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 4        | 0.3           |
| (1,2156) | 1:77:B:ASN:H     | 1:114:B:ARG:HA   | 8        | 0.3           |
| (1,2001) | 1:79:A:TYR:H     | 1:111:A:VAL:HA   | 16       | 0.3           |
| (1,1777) | 1:20:A:VAL:H     | 1:20:A:VAL:HG12  | 6        | 0.3           |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG21  | 16       | 0.3           |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG23 | 15       | 0.3           |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG23 | 15       | 0.3           |
| (1,1578) | 1:45:B:ASN:HD21  | 1:44:B:ILE:HA    | 5        | 0.3           |
| (1,1446) | 1:25:B:LYS:HE3   | 1:25:B:LYS:HG2   | 4        | 0.3           |
| (1,1445) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HG2   | 4        | 0.3           |
| (1,1387) | 1:20:A:VAL:HG12  | 1:19:A:SER:H     | 4        | 0.3           |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22  | 4        | 0.3           |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG23  | 19       | 0.3           |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG23  | 19       | 0.3           |
| (1,1224) | 1:20:B:VAL:HB    | 1:20:B:VAL:HG12  | 17       | 0.3           |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 10       | 0.3           |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG11  | 12       | 0.3           |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG12  | 17       | 0.3           |
| (1,1223) | 1:20:A:VAL:HB    | 1:20:A:VAL:HG13  | 19       | 0.3           |
| (1,1204) | 1:37:B:MET:HE2   | 1:26:B:THR:HG21  | 15       | 0.3           |
| (1,1203) | 1:37:A:MET:HE2   | 1:26:A:THR:HG21  | 15       | 0.3           |
| (1,987)  | 1:27:A:THR:HG21  | 1:35:A:GLU:HG3   | 15       | 0.3           |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG21  | 5        | 0.3           |
| (1,596)  | 1:107:B:ALA:HB3  | 1:106:B:THR:HA   | 5        | 0.3           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,595) | 1:107:A:ALA:HB3  | 1:106:A:THR:HA   | 5        | 0.3           |
| (1,542) | 1:92:B:MET:HE1   | 1:39:B:LEU:HD11  | 9        | 0.3           |
| (1,542) | 1:92:B:MET:HE3   | 1:39:B:LEU:HD12  | 18       | 0.3           |
| (1,541) | 1:92:A:MET:HE1   | 1:39:A:LEU:HD11  | 9        | 0.3           |
| (1,541) | 1:92:A:MET:HE3   | 1:39:A:LEU:HD12  | 18       | 0.3           |
| (1,460) | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 16       | 0.3           |
| (1,460) | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 18       | 0.3           |
| (1,459) | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 16       | 0.3           |
| (1,459) | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 18       | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 1        | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 2        | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 5        | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 6        | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD12 | 9        | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 11       | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD11 | 13       | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD12 | 17       | 0.3           |
| (1,386) | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD12 | 19       | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 1        | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 2        | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 5        | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 6        | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 11       | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 12       | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD11 | 13       | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD12 | 17       | 0.3           |
| (1,385) | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD12 | 19       | 0.3           |
| (1,364) | 1:117:B:VAL:HB   | 1:117:B:VAL:HG11 | 4        | 0.3           |
| (1,363) | 1:117:A:VAL:HB   | 1:117:A:VAL:HG11 | 4        | 0.3           |
| (1,344) | 1:48:B:VAL:HG12  | 1:41:B:GLU:HG2   | 15       | 0.3           |
| (1,343) | 1:48:A:VAL:HG12  | 1:41:A:GLU:HG2   | 15       | 0.3           |
| (1,252) | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 18       | 0.3           |
| (1,251) | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 18       | 0.3           |
| (1,238) | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 2        | 0.3           |
| (1,158) | 1:40:B:GLY:HA2   | 1:41:B:GLU:HG2   | 8        | 0.3           |
| (1,134) | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 9        | 0.3           |
| (1,133) | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 9        | 0.3           |
| (1,133) | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 15       | 0.3           |
| (1,88)  | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 1        | 0.3           |
| (1,88)  | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 2        | 0.3           |
| (1,88)  | 1:27:B:THR:HB    | 1:28:B:ALA:HB2   | 15       | 0.3           |
| (1,87)  | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 1        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 2        | 0.3           |
| (1,48)   | 1:42:B:VAL:HG22  | 1:44:B:ILE:HB    | 8        | 0.3           |
| (1,47)   | 1:42:A:VAL:HG22  | 1:44:A:ILE:HB    | 8        | 0.3           |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG22 | 7        | 0.3           |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG22 | 7        | 0.3           |
| (1,3072) | 1:44:B:ILE:HD11  | 1:99:A:TRP:HE1   | 11       | 0.29          |
| (1,3071) | 1:44:A:ILE:HD11  | 1:99:B:TRP:HE1   | 11       | 0.29          |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG13 | 6        | 0.29          |
| (1,3040) | 1:35:B:GLU:H     | 1:34:B:LYS:HD3   | 17       | 0.29          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 3        | 0.29          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 3        | 0.29          |
| (1,2770) | 1:18:B:VAL:H     | 1:57:B:LYS:HB2   | 14       | 0.29          |
| (1,2769) | 1:18:A:VAL:H     | 1:57:A:LYS:HB2   | 14       | 0.29          |
| (1,2560) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD13 | 6        | 0.29          |
| (1,2559) | 1:76:A:TRP:HE1   | 1:112:A:LEU:HD13 | 6        | 0.29          |
| (1,2544) | 1:76:B:TRP:HE1   | 1:112:B:LEU:HD21 | 2        | 0.29          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB1   | 4        | 0.29          |
| (1,2386) | 1:29:B:THR:H     | 1:29:B:THR:HG23  | 20       | 0.29          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG12 | 18       | 0.29          |
| (1,2155) | 1:77:A:ASN:H     | 1:114:A:ARG:HA   | 8        | 0.29          |
| (1,2002) | 1:79:B:TYR:H     | 1:111:B:VAL:HA   | 16       | 0.29          |
| (1,1880) | 1:21:B:TRP:H     | 1:20:B:VAL:HG21  | 2        | 0.29          |
| (1,1872) | 1:21:B:TRP:HE1   | 1:21:B:TRP:H     | 4        | 0.29          |
| (1,1871) | 1:21:A:TRP:HE1   | 1:21:A:TRP:H     | 4        | 0.29          |
| (1,1778) | 1:20:B:VAL:H     | 1:20:B:VAL:HG12  | 6        | 0.29          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG22  | 11       | 0.29          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG21  | 16       | 0.29          |
| (1,1388) | 1:20:B:VAL:HG12  | 1:19:B:SER:H     | 9        | 0.29          |
| (1,1387) | 1:20:A:VAL:HG12  | 1:19:A:SER:H     | 9        | 0.29          |
| (1,1384) | 1:18:B:VAL:HG21  | 1:59:B:ARG:HG2   | 8        | 0.29          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22  | 13       | 0.29          |
| (1,1170) | 1:39:B:LEU:HD11  | 1:92:B:MET:HG2   | 7        | 0.29          |
| (1,1170) | 1:39:B:LEU:HD13  | 1:92:B:MET:HG2   | 12       | 0.29          |
| (1,1169) | 1:39:A:LEU:HD11  | 1:92:A:MET:HG2   | 7        | 0.29          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 13       | 0.29          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 13       | 0.29          |
| (1,604)  | 1:104:B:ILE:HB   | 1:85:B:THR:HG21  | 5        | 0.29          |
| (1,542)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD11  | 7        | 0.29          |
| (1,541)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD11  | 7        | 0.29          |
| (1,424)  | 1:87:B:VAL:HG12  | 1:53:B:PHE:HD1   | 9        | 0.29          |
| (1,423)  | 1:87:A:VAL:HG12  | 1:53:A:PHE:HD1   | 9        | 0.29          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 12       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 18       | 0.29          |
| (1,386)  | 1:102:B:ILE:HG12 | 1:102:B:ILE:HD13 | 20       | 0.29          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 18       | 0.29          |
| (1,385)  | 1:102:A:ILE:HG12 | 1:102:A:ILE:HD13 | 20       | 0.29          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 7        | 0.29          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 7        | 0.29          |
| (1,194)  | 1:81:B:THR:HG21  | 1:79:B:TYR:HE1   | 17       | 0.29          |
| (1,193)  | 1:81:A:THR:HG21  | 1:79:A:TYR:HE1   | 17       | 0.29          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 2        | 0.29          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 3        | 0.29          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 6        | 0.29          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 14       | 0.29          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 2        | 0.29          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 3        | 0.29          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 6        | 0.29          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 14       | 0.29          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB3   | 4        | 0.29          |
| (1,61)   | 1:63:A:PRO:HD2   | 1:64:A:VAL:HG12  | 6        | 0.29          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 15       | 0.28          |
| (1,3100) | 1:9:B:ARG:HB3    | 1:117:A:VAL:HG23 | 12       | 0.28          |
| (1,3039) | 1:35:A:GLU:H     | 1:34:A:LYS:HD3   | 17       | 0.28          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 6        | 0.28          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 6        | 0.28          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB2  | 5        | 0.28          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB1  | 16       | 0.28          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB2  | 5        | 0.28          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB1  | 16       | 0.28          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG21 | 6        | 0.28          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG21 | 6        | 0.28          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB1   | 4        | 0.28          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 5        | 0.28          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB3   | 15       | 0.28          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB1   | 16       | 0.28          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 5        | 0.28          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB3   | 15       | 0.28          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB1   | 16       | 0.28          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 17       | 0.28          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG12 | 18       | 0.28          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 11       | 0.28          |
| (1,2196) | 1:55:B:GLU:H     | 1:22:B:VAL:HG12  | 19       | 0.28          |
| (1,2195) | 1:55:A:GLU:H     | 1:22:A:VAL:HG12  | 19       | 0.28          |
| (1,1879) | 1:21:A:TRP:H     | 1:20:A:VAL:HG21  | 2        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG22  | 11       | 0.28          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 16       | 0.28          |
| (1,1710) | 1:76:B:TRP:H     | 1:71:B:ILE:HG21  | 17       | 0.28          |
| (1,1709) | 1:76:A:TRP:H     | 1:71:A:ILE:HG21  | 17       | 0.28          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 4        | 0.28          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 17       | 0.28          |
| (1,1449) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HE1   | 4        | 0.28          |
| (1,1449) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HE1   | 17       | 0.28          |
| (1,1383) | 1:18:A:VAL:HG21  | 1:59:A:ARG:HG2   | 8        | 0.28          |
| (1,1362) | 1:104:B:ILE:HB   | 1:87:B:VAL:HG22  | 12       | 0.28          |
| (1,1361) | 1:104:A:ILE:HB   | 1:87:A:VAL:HG22  | 12       | 0.28          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG21  | 1        | 0.28          |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22  | 13       | 0.28          |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG21  | 1        | 0.28          |
| (1,1208) | 1:37:B:MET:HB2   | 1:26:B:THR:HG21  | 20       | 0.28          |
| (1,1207) | 1:37:A:MET:HB2   | 1:26:A:THR:HG21  | 20       | 0.28          |
| (1,1188) | 1:31:B:ILE:HD13  | 1:101:B:PHE:HB2  | 7        | 0.28          |
| (1,1187) | 1:31:A:ILE:HD13  | 1:101:A:PHE:HB2  | 7        | 0.28          |
| (1,1169) | 1:39:A:LEU:HD13  | 1:92:A:MET:HG2   | 12       | 0.28          |
| (1,1162) | 1:95:B:LYS:H     | 1:95:B:LYS:HE3   | 19       | 0.28          |
| (1,1161) | 1:95:A:LYS:H     | 1:95:A:LYS:HE3   | 19       | 0.28          |
| (1,988)  | 1:27:B:THR:HG21  | 1:35:B:GLU:HG3   | 15       | 0.28          |
| (1,926)  | 1:111:B:VAL:HG11 | 1:79:B:TYR:HE1   | 10       | 0.28          |
| (1,925)  | 1:111:A:VAL:HG11 | 1:79:A:TYR:HE1   | 10       | 0.28          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 1        | 0.28          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 1        | 0.28          |
| (1,604)  | 1:104:B:ILE:HB   | 1:85:B:THR:HG23  | 20       | 0.28          |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG23  | 20       | 0.28          |
| (1,596)  | 1:107:B:ALA:HB1  | 1:106:B:THR:HA   | 3        | 0.28          |
| (1,595)  | 1:107:A:ALA:HB1  | 1:106:A:THR:HA   | 3        | 0.28          |
| (1,541)  | 1:92:A:MET:HE2   | 1:39:A:LEU:HD11  | 14       | 0.28          |
| (1,453)  | 1:95:A:LYS:HB2   | 1:95:A:LYS:HD2   | 2        | 0.28          |
| (1,404)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG21 | 2        | 0.28          |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG22 | 18       | 0.28          |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG22 | 18       | 0.28          |
| (1,402)  | 1:102:B:ILE:HD12 | 1:25:B:LYS:HG2   | 3        | 0.28          |
| (1,401)  | 1:102:A:ILE:HD12 | 1:25:A:LYS:HG2   | 3        | 0.28          |
| (1,370)  | 1:114:B:ARG:HB2  | 1:76:B:TRP:HE3   | 7        | 0.28          |
| (1,369)  | 1:114:A:ARG:HB2  | 1:76:A:TRP:HE3   | 7        | 0.28          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 1        | 0.28          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 1        | 0.28          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 7        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 8        | 0.28          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 12       | 0.28          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 13       | 0.28          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 16       | 0.28          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 17       | 0.28          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 18       | 0.28          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 7        | 0.28          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 8        | 0.28          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 12       | 0.28          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 13       | 0.28          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 16       | 0.28          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 17       | 0.28          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 18       | 0.28          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB3   | 4        | 0.28          |
| (1,88)   | 1:27:B:THR:HB    | 1:28:B:ALA:HB1   | 8        | 0.28          |
| (1,87)   | 1:27:A:THR:HB    | 1:28:A:ALA:HB1   | 8        | 0.28          |
| (1,62)   | 1:63:B:PRO:HD2   | 1:64:B:VAL:HG12  | 6        | 0.28          |
| (1,54)   | 1:42:B:VAL:HG23  | 1:99:B:TRP:HZ2   | 4        | 0.28          |
| (1,53)   | 1:42:A:VAL:HG23  | 1:99:A:TRP:HZ2   | 4        | 0.28          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H     | 3        | 0.27          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H     | 12       | 0.27          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H     | 15       | 0.27          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 3        | 0.27          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 12       | 0.27          |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 17       | 0.27          |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 17       | 0.27          |
| (1,3088) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HA    | 6        | 0.27          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB2  | 10       | 0.27          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB3  | 12       | 0.27          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 10       | 0.27          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 7        | 0.27          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 7        | 0.27          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 12       | 0.27          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 12       | 0.27          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 13       | 0.27          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 13       | 0.27          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 13       | 0.27          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 14       | 0.27          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 14       | 0.27          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB3  | 3        | 0.27          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 10       | 0.27          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 17       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2330) | 1:75:B:HIS:H     | 1:74:B:LYS:H     | 7        | 0.27          |
| (1,2329) | 1:75:A:HIS:H     | 1:74:A:LYS:H     | 7        | 0.27          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG13 | 6        | 0.27          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG13 | 6        | 0.27          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 18       | 0.27          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 11       | 0.27          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2  | 1        | 0.27          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 1        | 0.27          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 7        | 0.27          |
| (1,2108) | 1:117:B:VAL:H    | 1:117:B:VAL:HB   | 20       | 0.27          |
| (1,2107) | 1:117:A:VAL:H    | 1:117:A:VAL:HB   | 20       | 0.27          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 1        | 0.27          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 1        | 0.27          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG23  | 18       | 0.27          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 16       | 0.27          |
| (1,1348) | 1:87:B:VAL:HG12  | 1:104:B:ILE:HD11 | 7        | 0.27          |
| (1,1347) | 1:87:A:VAL:HG12  | 1:104:A:ILE:HD11 | 7        | 0.27          |
| (1,1216) | 1:22:B:VAL:HG11  | 1:20:B:VAL:HB    | 3        | 0.27          |
| (1,1215) | 1:22:A:VAL:HG11  | 1:20:A:VAL:HB    | 3        | 0.27          |
| (1,874)  | 1:39:B:LEU:HD13  | 1:91:B:THR:HA    | 11       | 0.27          |
| (1,873)  | 1:39:A:LEU:HD13  | 1:91:A:THR:HA    | 11       | 0.27          |
| (1,542)  | 1:92:B:MET:HE2   | 1:39:B:LEU:HD11  | 14       | 0.27          |
| (1,541)  | 1:92:A:MET:HE3   | 1:39:A:LEU:HD11  | 15       | 0.27          |
| (1,454)  | 1:95:B:LYS:HB2   | 1:95:B:LYS:HD2   | 2        | 0.27          |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG21 | 14       | 0.27          |
| (1,403)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG21 | 2        | 0.27          |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG21 | 14       | 0.27          |
| (1,258)  | 1:112:B:LEU:HD21 | 1:76:B:TRP:HB2   | 14       | 0.27          |
| (1,257)  | 1:112:A:LEU:HD21 | 1:76:A:TRP:HB2   | 14       | 0.27          |
| (1,252)  | 1:112:B:LEU:HD23 | 1:71:B:ILE:HA    | 11       | 0.27          |
| (1,251)  | 1:112:A:LEU:HD23 | 1:71:A:ILE:HA    | 11       | 0.27          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 1        | 0.27          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 5        | 0.27          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 10       | 0.27          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 11       | 0.27          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 19       | 0.27          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 20       | 0.27          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 1        | 0.27          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 5        | 0.27          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 10       | 0.27          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 11       | 0.27          |
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 19       | 0.27          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,133)  | 1:39:A:LEU:HG  | 1:39:A:LEU:HB2   | 20       | 0.27          |
| (1,88)   | 1:27:B:THR:HB  | 1:28:B:ALA:HB1   | 14       | 0.27          |
| (1,88)   | 1:27:B:THR:HB  | 1:28:B:ALA:HB1   | 18       | 0.27          |
| (1,87)   | 1:27:A:THR:HB  | 1:28:A:ALA:HB1   | 14       | 0.27          |
| (1,87)   | 1:27:A:THR:HB  | 1:28:A:ALA:HB1   | 18       | 0.27          |
| (1,5)    | 1:79:A:TYR:H   | 1:111:A:VAL:HG21 | 15       | 0.27          |
| (3,16)   | 1:28:B:ALA:H   | 1:35:B:GLU:H     | 8        | 0.26          |
| (3,16)   | 1:28:B:ALA:H   | 1:35:B:GLU:H     | 14       | 0.26          |
| (3,15)   | 1:28:A:ALA:H   | 1:35:A:GLU:H     | 2        | 0.26          |
| (1,3099) | 1:9:A:ARG:HB3  | 1:117:B:VAL:HG23 | 12       | 0.26          |
| (1,3069) | 1:11:A:GLU:H   | 1:113:B:SER:HB3  | 12       | 0.26          |
| (1,3028) | 1:35:B:GLU:H   | 1:36:B:VAL:HG11  | 3        | 0.26          |
| (1,3027) | 1:35:A:GLU:H   | 1:36:A:VAL:HG11  | 3        | 0.26          |
| (1,2988) | 1:103:B:ARG:H  | 1:102:B:ILE:HG13 | 13       | 0.26          |
| (1,2905) | 1:22:A:VAL:H   | 1:53:A:PHE:HB3   | 1        | 0.26          |
| (1,2770) | 1:18:B:VAL:H   | 1:57:B:LYS:HB2   | 3        | 0.26          |
| (1,2769) | 1:18:A:VAL:H   | 1:57:A:LYS:HB2   | 3        | 0.26          |
| (1,2763) | 1:18:A:VAL:H   | 1:108:A:CYS:HB3  | 18       | 0.26          |
| (1,2608) | 1:107:B:ALA:H  | 1:56:B:THR:HG22  | 11       | 0.26          |
| (1,2588) | 1:107:B:ALA:H  | 1:107:B:ALA:HB3  | 3        | 0.26          |
| (1,2556) | 1:76:B:TRP:HE1 | 1:112:B:LEU:HB2  | 6        | 0.26          |
| (1,2555) | 1:76:A:TRP:HE1 | 1:112:A:LEU:HB2  | 6        | 0.26          |
| (1,2501) | 1:69:A:ARG:H   | 1:64:A:VAL:HG12  | 6        | 0.26          |
| (1,2388) | 1:29:B:THR:H   | 1:28:B:ALA:HB2   | 10       | 0.26          |
| (1,2386) | 1:29:B:THR:H   | 1:29:B:THR:HG21  | 19       | 0.26          |
| (1,2385) | 1:29:A:THR:H   | 1:29:A:THR:HG21  | 19       | 0.26          |
| (1,2228) | 1:118:B:ARG:H  | 1:117:B:VAL:HA   | 1        | 0.26          |
| (1,2228) | 1:118:B:ARG:H  | 1:117:B:VAL:HA   | 5        | 0.26          |
| (1,2227) | 1:118:A:ARG:H  | 1:117:A:VAL:HA   | 1        | 0.26          |
| (1,2227) | 1:118:A:ARG:H  | 1:117:A:VAL:HA   | 5        | 0.26          |
| (1,2227) | 1:118:A:ARG:H  | 1:117:A:VAL:HA   | 18       | 0.26          |
| (1,2224) | 1:118:B:ARG:H  | 1:118:B:ARG:HB2  | 7        | 0.26          |
| (1,2076) | 1:88:B:LYS:H   | 1:88:B:LYS:HG2   | 20       | 0.26          |
| (1,2075) | 1:88:A:LYS:H   | 1:88:A:LYS:HG2   | 20       | 0.26          |
| (1,1739) | 1:36:A:VAL:H   | 1:27:A:THR:HG23  | 18       | 0.26          |
| (1,1450) | 1:25:B:LYS:HG2 | 1:53:B:PHE:HE1   | 3        | 0.26          |
| (1,1449) | 1:25:A:LYS:HG2 | 1:53:A:PHE:HE1   | 3        | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2 | 1:25:B:LYS:HG2   | 1        | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2 | 1:25:B:LYS:HG2   | 3        | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2 | 1:25:B:LYS:HG2   | 7        | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2 | 1:25:B:LYS:HG2   | 8        | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2 | 1:25:B:LYS:HG2   | 11       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 13       | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 14       | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 15       | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 17       | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 18       | 0.26          |
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 19       | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 1        | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 3        | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 7        | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 8        | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 11       | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 13       | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 14       | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 15       | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 17       | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 18       | 0.26          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 19       | 0.26          |
| (1,1390) | 1:57:B:LYS:HE2   | 1:18:B:VAL:HG13  | 4        | 0.26          |
| (1,1389) | 1:57:A:LYS:HE2   | 1:18:A:VAL:HG13  | 4        | 0.26          |
| (1,1298) | 1:36:B:VAL:HG22  | 1:91:B:THR:H     | 20       | 0.26          |
| (1,1297) | 1:36:A:VAL:HG22  | 1:91:A:THR:H     | 20       | 0.26          |
| (1,1247) | 1:71:A:ILE:HG12  | 1:70:A:GLY:HA3   | 17       | 0.26          |
| (1,988)  | 1:27:B:THR:HG22  | 1:35:B:GLU:HG3   | 11       | 0.26          |
| (1,987)  | 1:27:A:THR:HG22  | 1:35:A:GLU:HG3   | 11       | 0.26          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB1  | 18       | 0.26          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB1  | 18       | 0.26          |
| (1,604)  | 1:104:B:ILE:HB   | 1:85:B:THR:HG22  | 4        | 0.26          |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG22  | 4        | 0.26          |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG22  | 17       | 0.26          |
| (1,588)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HB3  | 17       | 0.26          |
| (1,587)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HB3  | 17       | 0.26          |
| (1,542)  | 1:92:B:MET:HE3   | 1:39:B:LEU:HD11  | 15       | 0.26          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2   | 7        | 0.26          |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG21 | 5        | 0.26          |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG21 | 5        | 0.26          |
| (1,400)  | 1:102:B:ILE:HD12 | 1:87:B:VAL:HG22  | 2        | 0.26          |
| (1,399)  | 1:102:A:ILE:HD12 | 1:87:A:VAL:HG22  | 2        | 0.26          |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE3   | 18       | 0.26          |
| (1,281)  | 1:37:A:MET:HA    | 1:37:A:MET:HE3   | 18       | 0.26          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 10       | 0.26          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 10       | 0.26          |
| (1,134)  | 1:39:B:LEU:HG    | 1:39:B:LEU:HB2   | 4        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,133)  | 1:39:A:LEU:HG    | 1:39:A:LEU:HB2   | 4        | 0.26          |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG21 | 15       | 0.26          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H     | 2        | 0.25          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 8        | 0.25          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 14       | 0.25          |
| (1,3070) | 1:11:B:GLU:H     | 1:113:A:SER:HB3  | 16       | 0.25          |
| (1,3065) | 1:11:A:GLU:HA    | 1:111:B:VAL:HG13 | 6        | 0.25          |
| (1,3056) | 1:107:B:ALA:HB1  | 1:109:A:VAL:HG12 | 16       | 0.25          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 2        | 0.25          |
| (1,3033) | 1:35:A:GLU:H     | 1:34:A:LYS:HG3   | 2        | 0.25          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 17       | 0.25          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 17       | 0.25          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 1        | 0.25          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 2        | 0.25          |
| (1,2853) | 1:73:A:SER:H     | 1:76:A:TRP:HB3   | 2        | 0.25          |
| (1,2771) | 1:18:A:VAL:H     | 1:19:A:SER:HA    | 9        | 0.25          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 18       | 0.25          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG23  | 17       | 0.25          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG23  | 17       | 0.25          |
| (1,2607) | 1:107:A:ALA:H    | 1:56:A:THR:HG22  | 11       | 0.25          |
| (1,2597) | 1:107:A:ALA:H    | 1:108:A:CYS:HB3  | 13       | 0.25          |
| (1,2502) | 1:69:B:ARG:H     | 1:64:B:VAL:HG12  | 6        | 0.25          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 10       | 0.25          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 10       | 0.25          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 6        | 0.25          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 6        | 0.25          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2  | 6        | 0.25          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2  | 20       | 0.25          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 20       | 0.25          |
| (1,2107) | 1:117:A:VAL:H    | 1:117:A:VAL:HB   | 16       | 0.25          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 4        | 0.25          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 4        | 0.25          |
| (1,2014) | 1:79:B:TYR:H     | 1:111:B:VAL:HB   | 15       | 0.25          |
| (1,2013) | 1:79:A:TYR:H     | 1:111:A:VAL:HB   | 15       | 0.25          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG22  | 14       | 0.25          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG22  | 14       | 0.25          |
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 12       | 0.25          |
| (1,1444) | 1:25:B:LYS:HD2   | 1:25:B:LYS:HG2   | 20       | 0.25          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 12       | 0.25          |
| (1,1443) | 1:25:A:LYS:HD2   | 1:25:A:LYS:HG2   | 20       | 0.25          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG23  | 6        | 0.25          |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG23  | 6        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 1        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 2        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 3        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 4        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 5        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 6        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 7        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 9        | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 10       | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 11       | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 13       | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 14       | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 19       | 0.25          |
| (1,702) | 1:37:B:MET:HB2  | 1:37:B:MET:HB3  | 20       | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 1        | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 3        | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 4        | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 5        | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 7        | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 8        | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 9        | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 11       | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 13       | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 14       | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 15       | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 16       | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 18       | 0.25          |
| (1,701) | 1:37:A:MET:HB2  | 1:37:A:MET:HB3  | 19       | 0.25          |
| (1,604) | 1:104:B:ILE:HB  | 1:85:B:THR:HG22 | 17       | 0.25          |
| (1,583) | 1:115:A:LYS:HB2 | 1:115:A:LYS:HD2 | 17       | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 1        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 2        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 4        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 5        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 6        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 7        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 8        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 9        | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 11       | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 12       | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 14       | 0.25          |
| (1,484) | 1:32:B:LYS:HD2  | 1:32:B:LYS:HG2  | 15       | 0.25          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,484)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG2  | 16       | 0.25          |
| (1,484)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG2  | 17       | 0.25          |
| (1,484)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG2  | 19       | 0.25          |
| (1,484)  | 1:32:B:LYS:HD2   | 1:32:B:LYS:HG2  | 20       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 1        | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 2        | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 4        | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 5        | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 6        | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 8        | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 9        | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 11       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 12       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 14       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 15       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 16       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 17       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 19       | 0.25          |
| (1,483)  | 1:32:A:LYS:HD2   | 1:32:A:LYS:HG2  | 20       | 0.25          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3  | 9        | 0.25          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3  | 18       | 0.25          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3  | 9        | 0.25          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3  | 18       | 0.25          |
| (1,280)  | 1:88:B:LYS:HB2   | 1:88:B:LYS:HD2  | 10       | 0.25          |
| (1,279)  | 1:88:A:LYS:HB2   | 1:88:A:LYS:HD2  | 10       | 0.25          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23 | 1        | 0.25          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG22 | 3        | 0.25          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23 | 4        | 0.25          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG22 | 8        | 0.25          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG21 | 14       | 0.25          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG21 | 18       | 0.25          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23 | 19       | 0.25          |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23 | 1        | 0.25          |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG22 | 3        | 0.25          |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG22 | 8        | 0.25          |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG21 | 14       | 0.25          |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23 | 19       | 0.25          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA   | 17       | 0.25          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA   | 17       | 0.25          |
| (3,16)   | 1:28:B:ALA:H     | 1:35:B:GLU:H    | 11       | 0.24          |
| (1,3092) | 1:86:B:PHE:H     | 1:54:A:PHE:HD2  | 8        | 0.24          |
| (1,3087) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HA   | 18       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3072) | 1:44:B:ILE:HD13  | 1:99:A:TRP:HE1   | 15       | 0.24          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 10       | 0.24          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 1        | 0.24          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 1        | 0.24          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 7        | 0.24          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 7        | 0.24          |
| (1,2976) | 1:103:B:ARG:H    | 1:103:B:ARG:HG2  | 10       | 0.24          |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 10       | 0.24          |
| (1,2772) | 1:18:B:VAL:H     | 1:19:B:SER:HA    | 9        | 0.24          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 3        | 0.24          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 3        | 0.24          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 16       | 0.24          |
| (1,2604) | 1:107:B:ALA:H    | 1:82:B:THR:HA    | 5        | 0.24          |
| (1,2603) | 1:107:A:ALA:H    | 1:82:A:THR:HA    | 5        | 0.24          |
| (1,2598) | 1:107:B:ALA:H    | 1:108:B:CYS:HB3  | 13       | 0.24          |
| (1,2580) | 1:107:B:ALA:H    | 1:82:B:THR:HG23  | 14       | 0.24          |
| (1,2545) | 1:72:A:ASP:H     | 1:76:A:TRP:HE1   | 20       | 0.24          |
| (1,2466) | 1:6:B:ILE:H      | 1:6:B:ILE:HG13   | 11       | 0.24          |
| (1,2465) | 1:6:A:ILE:H      | 1:6:A:ILE:HG13   | 11       | 0.24          |
| (1,2431) | 1:92:A:MET:H     | 1:37:A:MET:HB2   | 1        | 0.24          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 18       | 0.24          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 18       | 0.24          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 13       | 0.24          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 13       | 0.24          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 6        | 0.24          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 2        | 0.24          |
| (1,2196) | 1:55:B:GLU:H     | 1:22:B:VAL:HG12  | 20       | 0.24          |
| (1,2195) | 1:55:A:GLU:H     | 1:22:A:VAL:HG12  | 20       | 0.24          |
| (1,2108) | 1:117:B:VAL:H    | 1:117:B:VAL:HB   | 6        | 0.24          |
| (1,2108) | 1:117:B:VAL:H    | 1:117:B:VAL:HB   | 13       | 0.24          |
| (1,2108) | 1:117:B:VAL:H    | 1:117:B:VAL:HB   | 16       | 0.24          |
| (1,2107) | 1:117:A:VAL:H    | 1:117:A:VAL:HB   | 6        | 0.24          |
| (1,1606) | 1:24:B:ASP:H     | 1:25:B:LYS:H     | 7        | 0.24          |
| (1,1605) | 1:24:A:ASP:H     | 1:25:A:LYS:H     | 7        | 0.24          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG21  | 15       | 0.24          |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG21  | 15       | 0.24          |
| (1,1248) | 1:71:B:ILE:HG12  | 1:70:B:GLY:HA3   | 17       | 0.24          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 1        | 0.24          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 1        | 0.24          |
| (1,988)  | 1:27:B:THR:HG23  | 1:35:B:GLU:HG3   | 17       | 0.24          |
| (1,987)  | 1:27:A:THR:HG23  | 1:35:A:GLU:HG3   | 17       | 0.24          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 5        | 0.24          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,702) | 1:37:B:MET:HB2   | 1:37:B:MET:HB3   | 8        | 0.24          |
| (1,702) | 1:37:B:MET:HB2   | 1:37:B:MET:HB3   | 12       | 0.24          |
| (1,702) | 1:37:B:MET:HB2   | 1:37:B:MET:HB3   | 15       | 0.24          |
| (1,702) | 1:37:B:MET:HB2   | 1:37:B:MET:HB3   | 16       | 0.24          |
| (1,702) | 1:37:B:MET:HB2   | 1:37:B:MET:HB3   | 17       | 0.24          |
| (1,702) | 1:37:B:MET:HB2   | 1:37:B:MET:HB3   | 18       | 0.24          |
| (1,701) | 1:37:A:MET:HB2   | 1:37:A:MET:HB3   | 2        | 0.24          |
| (1,701) | 1:37:A:MET:HB2   | 1:37:A:MET:HB3   | 6        | 0.24          |
| (1,701) | 1:37:A:MET:HB2   | 1:37:A:MET:HB3   | 10       | 0.24          |
| (1,701) | 1:37:A:MET:HB2   | 1:37:A:MET:HB3   | 12       | 0.24          |
| (1,701) | 1:37:A:MET:HB2   | 1:37:A:MET:HB3   | 17       | 0.24          |
| (1,701) | 1:37:A:MET:HB2   | 1:37:A:MET:HB3   | 20       | 0.24          |
| (1,682) | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 14       | 0.24          |
| (1,681) | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 14       | 0.24          |
| (1,584) | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 12       | 0.24          |
| (1,584) | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 17       | 0.24          |
| (1,461) | 1:44:A:ILE:HG12  | 1:43:A:ASN:HB2   | 1        | 0.24          |
| (1,416) | 1:39:B:LEU:H     | 1:38:B:VAL:HG13  | 3        | 0.24          |
| (1,415) | 1:39:A:LEU:H     | 1:38:A:VAL:HG13  | 3        | 0.24          |
| (1,404) | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG22 | 6        | 0.24          |
| (1,403) | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG22 | 6        | 0.24          |
| (1,344) | 1:48:B:VAL:HG13  | 1:41:B:GLU:HG2   | 4        | 0.24          |
| (1,300) | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 12       | 0.24          |
| (1,299) | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 12       | 0.24          |
| (1,240) | 1:20:B:VAL:HA    | 1:20:B:VAL:HG22  | 5        | 0.24          |
| (1,240) | 1:20:B:VAL:HA    | 1:20:B:VAL:HG21  | 12       | 0.24          |
| (1,240) | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23  | 15       | 0.24          |
| (1,240) | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23  | 16       | 0.24          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23  | 4        | 0.24          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG22  | 5        | 0.24          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG21  | 12       | 0.24          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23  | 15       | 0.24          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23  | 16       | 0.24          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG21  | 18       | 0.24          |
| (1,238) | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 8        | 0.24          |
| (1,237) | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 8        | 0.24          |
| (1,152) | 1:100:B:ARG:HG3  | 1:100:B:ARG:HG2  | 1        | 0.24          |
| (1,152) | 1:100:B:ARG:HG3  | 1:100:B:ARG:HG2  | 2        | 0.24          |
| (1,152) | 1:100:B:ARG:HG3  | 1:100:B:ARG:HG2  | 3        | 0.24          |
| (1,152) | 1:100:B:ARG:HG3  | 1:100:B:ARG:HG2  | 4        | 0.24          |
| (1,152) | 1:100:B:ARG:HG3  | 1:100:B:ARG:HG2  | 5        | 0.24          |
| (1,152) | 1:100:B:ARG:HG3  | 1:100:B:ARG:HG2  | 6        | 0.24          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 7        | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 8        | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 9        | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 10       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 11       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 12       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 13       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 14       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 15       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 16       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 17       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 18       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 19       | 0.24          |
| (1,152)  | 1:100:B:ARG:HG3 | 1:100:B:ARG:HG2  | 20       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 1        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 2        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 3        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 4        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 5        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 6        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 7        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 8        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 9        | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 10       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 11       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 12       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 13       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 14       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 15       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 16       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 17       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 18       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 19       | 0.24          |
| (1,151)  | 1:100:A:ARG:HG3 | 1:100:A:ARG:HG2  | 20       | 0.24          |
| (3,15)   | 1:28:A:ALA:H    | 1:35:A:GLU:H     | 11       | 0.23          |
| (1,3102) | 1:9:B:ARG:HB2   | 1:115:A:LYS:HA   | 9        | 0.23          |
| (1,3091) | 1:86:A:PHE:H    | 1:54:B:PHE:HD2   | 8        | 0.23          |
| (1,3065) | 1:11:A:GLU:HA   | 1:111:B:VAL:HG13 | 11       | 0.23          |
| (1,3055) | 1:107:A:ALA:HB1 | 1:109:B:VAL:HG13 | 11       | 0.23          |
| (1,3055) | 1:107:A:ALA:HB1 | 1:109:B:VAL:HG12 | 16       | 0.23          |
| (1,3033) | 1:35:A:GLU:H    | 1:34:A:LYS:HG3   | 7        | 0.23          |
| (1,3004) | 1:28:B:ALA:H    | 1:38:B:VAL:HG12  | 8        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG11  | 19       | 0.23          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG12  | 8        | 0.23          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG11  | 19       | 0.23          |
| (1,2976) | 1:103:B:ARG:H    | 1:103:B:ARG:HG2  | 16       | 0.23          |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 16       | 0.23          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 16       | 0.23          |
| (1,2579) | 1:107:A:ALA:H    | 1:82:A:THR:HG23  | 14       | 0.23          |
| (1,2546) | 1:72:B:ASP:H     | 1:76:B:TRP:HE1   | 20       | 0.23          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB3   | 9        | 0.23          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG13 | 5        | 0.23          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG13 | 5        | 0.23          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 2        | 0.23          |
| (1,2107) | 1:117:A:VAL:H    | 1:117:A:VAL:HB   | 13       | 0.23          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 3        | 0.23          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 6        | 0.23          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 18       | 0.23          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 3        | 0.23          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 6        | 0.23          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 11       | 0.23          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 14       | 0.23          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 18       | 0.23          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 17       | 0.23          |
| (1,2014) | 1:79:B:TYR:H     | 1:111:B:VAL:HB   | 6        | 0.23          |
| (1,2013) | 1:79:A:TYR:H     | 1:111:A:VAL:HB   | 6        | 0.23          |
| (1,1951) | 1:105:A:ASP:H    | 1:55:A:GLU:HB2   | 7        | 0.23          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG21  | 15       | 0.23          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 5        | 0.23          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 10       | 0.23          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG12  | 11       | 0.23          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 15       | 0.23          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 16       | 0.23          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 19       | 0.23          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 20       | 0.23          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 5        | 0.23          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 10       | 0.23          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG12  | 11       | 0.23          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 15       | 0.23          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 16       | 0.23          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 19       | 0.23          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG12  | 20       | 0.23          |
| (1,1354) | 1:104:B:ILE:HD11 | 1:87:B:VAL:HG21  | 5        | 0.23          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG23  | 20       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1353) | 1:104:A:ILE:HD11 | 1:87:A:VAL:HG21  | 5        | 0.23          |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG23  | 20       | 0.23          |
| (1,1348) | 1:87:B:VAL:HG11  | 1:104:B:ILE:HD11 | 11       | 0.23          |
| (1,1347) | 1:87:A:VAL:HG11  | 1:104:A:ILE:HD11 | 11       | 0.23          |
| (1,1331) | 1:64:A:VAL:HG23  | 1:65:A:ASP:HB3   | 16       | 0.23          |
| (1,1191) | 1:33:A:GLY:HA2   | 1:29:A:THR:HG21  | 12       | 0.23          |
| (1,1187) | 1:31:A:ILE:HD11  | 1:101:A:PHE:HB2  | 18       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 1        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 2        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 3        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 4        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 6        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 7        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 8        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 9        | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 10       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 11       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 12       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 13       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 14       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 15       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 16       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 17       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 18       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 19       | 0.23          |
| (1,972)  | 1:34:B:LYS:HG3   | 1:34:B:LYS:HD3   | 20       | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 1        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 2        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 3        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 4        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 5        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 6        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 7        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 8        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 9        | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 10       | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 11       | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 12       | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 13       | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 14       | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 15       | 0.23          |
| (1,971)  | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 16       | 0.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,971) | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 17       | 0.23          |
| (1,971) | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 18       | 0.23          |
| (1,971) | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 19       | 0.23          |
| (1,971) | 1:34:A:LYS:HG3   | 1:34:A:LYS:HD3   | 20       | 0.23          |
| (1,938) | 1:97:B:ALA:HB3   | 1:90:B:LEU:HD21  | 4        | 0.23          |
| (1,854) | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 19       | 0.23          |
| (1,853) | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 19       | 0.23          |
| (1,806) | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 4        | 0.23          |
| (1,806) | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 5        | 0.23          |
| (1,806) | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 11       | 0.23          |
| (1,805) | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 4        | 0.23          |
| (1,805) | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 5        | 0.23          |
| (1,805) | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 11       | 0.23          |
| (1,802) | 1:59:B:ARG:HB3   | 1:59:B:ARG:HG2   | 15       | 0.23          |
| (1,801) | 1:59:A:ARG:HB3   | 1:59:A:ARG:HG2   | 15       | 0.23          |
| (1,682) | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 11       | 0.23          |
| (1,681) | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 11       | 0.23          |
| (1,583) | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 12       | 0.23          |
| (1,583) | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 18       | 0.23          |
| (1,462) | 1:44:B:ILE:HG12  | 1:43:B:ASN:HB2   | 1        | 0.23          |
| (1,426) | 1:87:B:VAL:HG12  | 1:53:B:PHE:HE1   | 9        | 0.23          |
| (1,425) | 1:87:A:VAL:HG12  | 1:53:A:PHE:HE1   | 9        | 0.23          |
| (1,416) | 1:39:B:LEU:H     | 1:38:B:VAL:HG11  | 11       | 0.23          |
| (1,416) | 1:39:B:LEU:H     | 1:38:B:VAL:HG12  | 12       | 0.23          |
| (1,415) | 1:39:A:LEU:H     | 1:38:A:VAL:HG12  | 12       | 0.23          |
| (1,404) | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG23 | 10       | 0.23          |
| (1,404) | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG21 | 12       | 0.23          |
| (1,403) | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG23 | 10       | 0.23          |
| (1,403) | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG21 | 12       | 0.23          |
| (1,403) | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG22 | 19       | 0.23          |
| (1,343) | 1:48:A:VAL:HG13  | 1:41:A:GLU:HG2   | 4        | 0.23          |
| (1,300) | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 1        | 0.23          |
| (1,300) | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 17       | 0.23          |
| (1,299) | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 1        | 0.23          |
| (1,299) | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 17       | 0.23          |
| (1,280) | 1:88:B:LYS:HB2   | 1:88:B:LYS:HD2   | 4        | 0.23          |
| (1,279) | 1:88:A:LYS:HB2   | 1:88:A:LYS:HD2   | 4        | 0.23          |
| (1,240) | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23  | 7        | 0.23          |
| (1,240) | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23  | 11       | 0.23          |
| (1,240) | 1:20:B:VAL:HA    | 1:20:B:VAL:HG21  | 13       | 0.23          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23  | 7        | 0.23          |
| (1,239) | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23  | 11       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG21  | 13       | 0.23          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 18       | 0.23          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 12       | 0.23          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 18       | 0.23          |
| (1,47)   | 1:42:A:VAL:HG21  | 1:44:A:ILE:HB    | 2        | 0.23          |
| (1,4)    | 1:111:B:VAL:HG22 | 1:112:B:LEU:HD23 | 14       | 0.23          |
| (1,3)    | 1:111:A:VAL:HG22 | 1:112:A:LEU:HD23 | 14       | 0.23          |
| (1,3080) | 1:11:B:GLU:HG2   | 1:111:A:VAL:HG23 | 2        | 0.22          |
| (1,3071) | 1:44:A:ILE:HD13  | 1:99:B:TRP:HE1   | 15       | 0.22          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB2  | 10       | 0.22          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB3  | 16       | 0.22          |
| (1,3056) | 1:107:B:ALA:HB1  | 1:109:A:VAL:HG13 | 11       | 0.22          |
| (1,3034) | 1:35:B:GLU:H     | 1:34:B:LYS:HG3   | 7        | 0.22          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 10       | 0.22          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 10       | 0.22          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 16       | 0.22          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 1        | 0.22          |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 1        | 0.22          |
| (1,2976) | 1:103:B:ARG:H    | 1:103:B:ARG:HG2  | 12       | 0.22          |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 12       | 0.22          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 2        | 0.22          |
| (1,2906) | 1:22:B:VAL:H     | 1:53:B:PHE:HB3   | 12       | 0.22          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 2        | 0.22          |
| (1,2905) | 1:22:A:VAL:H     | 1:53:A:PHE:HB3   | 12       | 0.22          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB1  | 14       | 0.22          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB3  | 20       | 0.22          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB3  | 20       | 0.22          |
| (1,2432) | 1:92:B:MET:H     | 1:37:B:MET:HB2   | 1        | 0.22          |
| (1,2390) | 1:29:B:THR:H     | 1:102:B:ILE:HG23 | 15       | 0.22          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG23 | 15       | 0.22          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 17       | 0.22          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB3   | 9        | 0.22          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 15       | 0.22          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 15       | 0.22          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG13 | 7        | 0.22          |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG13 | 7        | 0.22          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 10       | 0.22          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2  | 3        | 0.22          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 3        | 0.22          |
| (1,2107) | 1:117:A:VAL:H    | 1:117:A:VAL:HB   | 15       | 0.22          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 1        | 0.22          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 5        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 9        | 0.22          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 11       | 0.22          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 14       | 0.22          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 5        | 0.22          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 9        | 0.22          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 17       | 0.22          |
| (1,1996) | 1:67:B:GLY:H     | 1:64:B:VAL:HB    | 13       | 0.22          |
| (1,1995) | 1:67:A:GLY:H     | 1:64:A:VAL:HB    | 13       | 0.22          |
| (1,1952) | 1:105:B:ASP:H    | 1:55:B:GLU:HB2   | 7        | 0.22          |
| (1,1880) | 1:21:B:TRP:H     | 1:20:B:VAL:HG22  | 16       | 0.22          |
| (1,1879) | 1:21:A:TRP:H     | 1:20:A:VAL:HG22  | 16       | 0.22          |
| (1,1778) | 1:20:B:VAL:H     | 1:20:B:VAL:HG11  | 20       | 0.22          |
| (1,1777) | 1:20:A:VAL:H     | 1:20:A:VAL:HG11  | 20       | 0.22          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG21  | 3        | 0.22          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG21  | 15       | 0.22          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG21  | 3        | 0.22          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG21 | 17       | 0.22          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG21 | 17       | 0.22          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG21 | 7        | 0.22          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG23 | 9        | 0.22          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG21 | 10       | 0.22          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 11       | 0.22          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 13       | 0.22          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 19       | 0.22          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG21 | 7        | 0.22          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG23 | 9        | 0.22          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG21 | 10       | 0.22          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG21 | 13       | 0.22          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 19       | 0.22          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG21  | 20       | 0.22          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG21  | 20       | 0.22          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 1        | 0.22          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 3        | 0.22          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG12  | 8        | 0.22          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 9        | 0.22          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 13       | 0.22          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG12  | 17       | 0.22          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 1        | 0.22          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 3        | 0.22          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG12  | 8        | 0.22          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 9        | 0.22          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 13       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG12  | 17       | 0.22          |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG21  | 16       | 0.22          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG21  | 16       | 0.22          |
| (1,1348) | 1:87:B:VAL:HG12  | 1:104:B:ILE:HD12 | 18       | 0.22          |
| (1,1347) | 1:87:A:VAL:HG12  | 1:104:A:ILE:HD12 | 18       | 0.22          |
| (1,1332) | 1:64:B:VAL:HG23  | 1:65:B:ASP:HB3   | 16       | 0.22          |
| (1,1192) | 1:33:B:GLY:HA2   | 1:29:B:THR:HG21  | 12       | 0.22          |
| (1,1188) | 1:31:B:ILE:HD11  | 1:101:B:PHE:HB2  | 18       | 0.22          |
| (1,1170) | 1:39:B:LEU:HD11  | 1:92:B:MET:HG2   | 15       | 0.22          |
| (1,1169) | 1:39:A:LEU:HD11  | 1:92:A:MET:HG2   | 15       | 0.22          |
| (1,988)  | 1:27:B:THR:HG21  | 1:35:B:GLU:HG3   | 16       | 0.22          |
| (1,987)  | 1:27:A:THR:HG21  | 1:35:A:GLU:HG3   | 16       | 0.22          |
| (1,937)  | 1:97:A:ALA:HB3   | 1:90:A:LEU:HD21  | 4        | 0.22          |
| (1,874)  | 1:39:B:LEU:HD12  | 1:91:B:THR:HA    | 10       | 0.22          |
| (1,873)  | 1:39:A:LEU:HD12  | 1:91:A:THR:HA    | 10       | 0.22          |
| (1,854)  | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 15       | 0.22          |
| (1,853)  | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 15       | 0.22          |
| (1,806)  | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 1        | 0.22          |
| (1,806)  | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 3        | 0.22          |
| (1,806)  | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 6        | 0.22          |
| (1,806)  | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 9        | 0.22          |
| (1,805)  | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 1        | 0.22          |
| (1,805)  | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 3        | 0.22          |
| (1,805)  | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 6        | 0.22          |
| (1,805)  | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 9        | 0.22          |
| (1,604)  | 1:104:B:ILE:HB   | 1:85:B:THR:HG22  | 16       | 0.22          |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG22  | 16       | 0.22          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 2        | 0.22          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 6        | 0.22          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 11       | 0.22          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 12       | 0.22          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 13       | 0.22          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 14       | 0.22          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 17       | 0.22          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 2        | 0.22          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 6        | 0.22          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 11       | 0.22          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 12       | 0.22          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 13       | 0.22          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 14       | 0.22          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 17       | 0.22          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 13       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 18       | 0.22          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 13       | 0.22          |
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG11  | 11       | 0.22          |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG21 | 16       | 0.22          |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG22 | 17       | 0.22          |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG22 | 19       | 0.22          |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG21 | 16       | 0.22          |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG22 | 17       | 0.22          |
| (1,343)  | 1:48:A:VAL:HG11  | 1:41:A:GLU:HG2   | 14       | 0.22          |
| (1,258)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HB2   | 3        | 0.22          |
| (1,257)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HB2   | 3        | 0.22          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG22  | 2        | 0.22          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG22  | 10       | 0.22          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23  | 17       | 0.22          |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG22  | 10       | 0.22          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 4        | 0.22          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 6        | 0.22          |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 12       | 0.22          |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 4        | 0.22          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 11       | 0.22          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 20       | 0.22          |
| (1,48)   | 1:42:B:VAL:HG21  | 1:44:B:ILE:HB    | 2        | 0.22          |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG23 | 5        | 0.22          |
| (1,6)    | 1:79:B:TYR:H     | 1:111:B:VAL:HG21 | 8        | 0.22          |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG21 | 8        | 0.22          |
| (1,3101) | 1:9:A:ARG:HB2    | 1:115:B:LYS:HA   | 9        | 0.21          |
| (1,3087) | 1:112:A:LEU:HD13 | 1:14:B:VAL:HA    | 13       | 0.21          |
| (1,3066) | 1:11:B:GLU:HA    | 1:111:A:VAL:HG13 | 11       | 0.21          |
| (1,3049) | 1:21:A:TRP:HH2   | 1:31:B:ILE:HD12  | 11       | 0.21          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 2        | 0.21          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 5        | 0.21          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 14       | 0.21          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 16       | 0.21          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 2        | 0.21          |
| (1,2866) | 1:74:B:LYS:H     | 1:73:B:SER:H     | 20       | 0.21          |
| (1,2840) | 1:74:B:LYS:H     | 1:72:B:ASP:HA    | 7        | 0.21          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 1        | 0.21          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB3  | 1        | 0.21          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB1  | 2        | 0.21          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB2  | 9        | 0.21          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB3  | 1        | 0.21          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB1  | 2        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB2  | 9        | 0.21          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB1  | 14       | 0.21          |
| (1,2428) | 1:92:B:MET:H     | 1:92:B:MET:HE3   | 8        | 0.21          |
| (1,2427) | 1:92:A:MET:H     | 1:92:A:MET:HE3   | 8        | 0.21          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 20       | 0.21          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 17       | 0.21          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 20       | 0.21          |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG13 | 3        | 0.21          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 10       | 0.21          |
| (1,2108) | 1:117:B:VAL:H    | 1:117:B:VAL:HB   | 15       | 0.21          |
| (1,2108) | 1:117:B:VAL:H    | 1:117:B:VAL:HB   | 19       | 0.21          |
| (1,2090) | 1:68:B:CYS:H     | 1:70:B:GLY:H     | 12       | 0.21          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 10       | 0.21          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 19       | 0.21          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 20       | 0.21          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 1        | 0.21          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 10       | 0.21          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 19       | 0.21          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 20       | 0.21          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 7        | 0.21          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 7        | 0.21          |
| (1,1542) | 1:54:B:PHE:HB2   | 1:55:B:GLU:HG3   | 2        | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG23 | 1        | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG21 | 3        | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG23 | 8        | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG21 | 12       | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG21 | 15       | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 16       | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 17       | 0.21          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 20       | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG23 | 1        | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG21 | 3        | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG23 | 8        | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 11       | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG21 | 12       | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG21 | 15       | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 16       | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 17       | 0.21          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 20       | 0.21          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 2        | 0.21          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 6        | 0.21          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 7        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG13  | 12       | 0.21          |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG12  | 18       | 0.21          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 2        | 0.21          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 6        | 0.21          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 7        | 0.21          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG13  | 12       | 0.21          |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG12  | 18       | 0.21          |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22  | 11       | 0.21          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG23  | 17       | 0.21          |
| (1,1348) | 1:87:B:VAL:HG11  | 1:104:B:ILE:HD11 | 12       | 0.21          |
| (1,1347) | 1:87:A:VAL:HG11  | 1:104:A:ILE:HD11 | 12       | 0.21          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 4        | 0.21          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 4        | 0.21          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 6        | 0.21          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 6        | 0.21          |
| (1,988)  | 1:27:B:THR:HG22  | 1:35:B:GLU:HG3   | 9        | 0.21          |
| (1,920)  | 1:117:B:VAL:HB   | 1:116:B:ALA:HB2  | 11       | 0.21          |
| (1,919)  | 1:117:A:VAL:HB   | 1:116:A:ALA:HB2  | 11       | 0.21          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 1        | 0.21          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 16       | 0.21          |
| (1,586)  | 1:115:B:LYS:HD2  | 1:115:B:LYS:HG2  | 18       | 0.21          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 1        | 0.21          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 16       | 0.21          |
| (1,585)  | 1:115:A:LYS:HD2  | 1:115:A:LYS:HG2  | 18       | 0.21          |
| (1,416)  | 1:39:B:LEU:H     | 1:38:B:VAL:HG13  | 6        | 0.21          |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG21 | 7        | 0.21          |
| (1,404)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG23 | 9        | 0.21          |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG21 | 15       | 0.21          |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG21 | 7        | 0.21          |
| (1,403)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG23 | 9        | 0.21          |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG21 | 15       | 0.21          |
| (1,344)  | 1:48:B:VAL:HG11  | 1:41:B:GLU:HG2   | 14       | 0.21          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 5        | 0.21          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 10       | 0.21          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 13       | 0.21          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 20       | 0.21          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 5        | 0.21          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 10       | 0.21          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 13       | 0.21          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 20       | 0.21          |
| (1,280)  | 1:88:B:LYS:HB2   | 1:88:B:LYS:HD2   | 16       | 0.21          |
| (1,279)  | 1:88:A:LYS:HB2   | 1:88:A:LYS:HD2   | 16       | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,240)  | 1:20:B:VAL:HA   | 1:20:B:VAL:HG22  | 20       | 0.21          |
| (1,239)  | 1:20:A:VAL:HA   | 1:20:A:VAL:HG22  | 2        | 0.21          |
| (1,239)  | 1:20:A:VAL:HA   | 1:20:A:VAL:HG23  | 17       | 0.21          |
| (1,239)  | 1:20:A:VAL:HA   | 1:20:A:VAL:HG22  | 20       | 0.21          |
| (1,237)  | 1:55:A:GLU:H    | 1:20:A:VAL:HA    | 6        | 0.21          |
| (1,68)   | 1:32:B:LYS:HE2  | 1:32:B:LYS:HG3   | 20       | 0.21          |
| (1,67)   | 1:32:A:LYS:HE2  | 1:32:A:LYS:HG3   | 11       | 0.21          |
| (1,67)   | 1:32:A:LYS:HE2  | 1:32:A:LYS:HG3   | 16       | 0.21          |
| (1,5)    | 1:79:A:TYR:H    | 1:111:A:VAL:HG23 | 5        | 0.21          |
| (3,16)   | 1:28:B:ALA:H    | 1:35:B:GLU:H     | 16       | 0.2           |
| (3,16)   | 1:28:B:ALA:H    | 1:103:B:ARG:H    | 19       | 0.2           |
| (3,15)   | 1:28:A:ALA:H    | 1:103:A:ARG:H    | 19       | 0.2           |
| (1,3053) | 1:70:A:GLY:HA3  | 1:112:B:LEU:HG   | 14       | 0.2           |
| (1,3014) | 1:28:B:ALA:H    | 1:29:B:THR:HA    | 17       | 0.2           |
| (1,3014) | 1:28:B:ALA:H    | 1:29:B:THR:HA    | 19       | 0.2           |
| (1,3013) | 1:28:A:ALA:H    | 1:29:A:THR:HA    | 5        | 0.2           |
| (1,3013) | 1:28:A:ALA:H    | 1:29:A:THR:HA    | 14       | 0.2           |
| (1,3013) | 1:28:A:ALA:H    | 1:29:A:THR:HA    | 17       | 0.2           |
| (1,3013) | 1:28:A:ALA:H    | 1:29:A:THR:HA    | 19       | 0.2           |
| (1,2865) | 1:74:A:LYS:H    | 1:73:A:SER:H     | 20       | 0.2           |
| (1,2764) | 1:18:B:VAL:H    | 1:108:B:CYS:HB3  | 1        | 0.2           |
| (1,2736) | 1:51:B:GLN:HE21 | 1:90:B:LEU:H     | 5        | 0.2           |
| (1,2735) | 1:51:A:GLN:HE21 | 1:90:A:LEU:H     | 5        | 0.2           |
| (1,2720) | 1:84:B:HIS:H    | 1:83:B:THR:HB    | 1        | 0.2           |
| (1,2720) | 1:84:B:HIS:H    | 1:83:B:THR:HB    | 15       | 0.2           |
| (1,2719) | 1:84:A:HIS:H    | 1:83:A:THR:HB    | 15       | 0.2           |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB3  | 10       | 0.2           |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB3  | 10       | 0.2           |
| (1,2388) | 1:29:B:THR:H    | 1:28:B:ALA:HB2   | 14       | 0.2           |
| (1,2384) | 1:29:B:THR:H    | 1:30:B:ASP:HB2   | 9        | 0.2           |
| (1,2383) | 1:29:A:THR:H    | 1:30:A:ASP:HB2   | 9        | 0.2           |
| (1,2253) | 1:77:A:ASN:HD22 | 1:114:A:ARG:HA   | 20       | 0.2           |
| (1,2232) | 1:118:B:ARG:H   | 1:117:B:VAL:HG12 | 11       | 0.2           |
| (1,2231) | 1:118:A:ARG:H   | 1:117:A:VAL:HG13 | 3        | 0.2           |
| (1,2231) | 1:118:A:ARG:H   | 1:117:A:VAL:HG12 | 11       | 0.2           |
| (1,2228) | 1:118:B:ARG:H   | 1:117:B:VAL:HA   | 16       | 0.2           |
| (1,2126) | 1:32:B:LYS:H    | 1:31:B:ILE:HG12  | 15       | 0.2           |
| (1,2125) | 1:32:A:LYS:H    | 1:31:A:ILE:HG12  | 15       | 0.2           |
| (1,2107) | 1:117:A:VAL:H   | 1:117:A:VAL:HB   | 19       | 0.2           |
| (1,2089) | 1:68:A:CYS:H    | 1:70:A:GLY:H     | 12       | 0.2           |
| (1,2046) | 1:27:B:THR:H    | 1:28:B:ALA:H     | 2        | 0.2           |
| (1,2046) | 1:27:B:THR:H    | 1:28:B:ALA:H     | 15       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 16       | 0.2           |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 15       | 0.2           |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 16       | 0.2           |
| (1,1910) | 1:72:B:ASP:H     | 1:71:B:ILE:HG21  | 10       | 0.2           |
| (1,1909) | 1:72:A:ASP:H     | 1:71:A:ILE:HG21  | 10       | 0.2           |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG22  | 9        | 0.2           |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG23  | 17       | 0.2           |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG23  | 17       | 0.2           |
| (1,1541) | 1:54:A:PHE:HB2   | 1:55:A:GLU:HG3   | 2        | 0.2           |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 2        | 0.2           |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG23 | 6        | 0.2           |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 14       | 0.2           |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 2        | 0.2           |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG23 | 6        | 0.2           |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 14       | 0.2           |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG12  | 4        | 0.2           |
| (1,1394) | 1:18:B:VAL:HB    | 1:18:B:VAL:HG11  | 14       | 0.2           |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG12  | 4        | 0.2           |
| (1,1393) | 1:18:A:VAL:HB    | 1:18:A:VAL:HG11  | 14       | 0.2           |
| (1,1392) | 1:59:B:ARG:HD2   | 1:18:B:VAL:HG11  | 12       | 0.2           |
| (1,1391) | 1:59:A:ARG:HD2   | 1:18:A:VAL:HG11  | 12       | 0.2           |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22  | 11       | 0.2           |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG23  | 17       | 0.2           |
| (1,1298) | 1:36:B:VAL:HG23  | 1:91:B:THR:H     | 6        | 0.2           |
| (1,1297) | 1:36:A:VAL:HG23  | 1:91:A:THR:H     | 6        | 0.2           |
| (1,988)  | 1:27:B:THR:HG22  | 1:35:B:GLU:HG3   | 12       | 0.2           |
| (1,987)  | 1:27:A:THR:HG21  | 1:35:A:GLU:HG3   | 6        | 0.2           |
| (1,987)  | 1:27:A:THR:HG22  | 1:35:A:GLU:HG3   | 9        | 0.2           |
| (1,987)  | 1:27:A:THR:HG22  | 1:35:A:GLU:HG3   | 12       | 0.2           |
| (1,854)  | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 7        | 0.2           |
| (1,853)  | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 7        | 0.2           |
| (1,806)  | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 7        | 0.2           |
| (1,805)  | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 7        | 0.2           |
| (1,712)  | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 2        | 0.2           |
| (1,711)  | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 2        | 0.2           |
| (1,604)  | 1:104:B:ILE:HB   | 1:85:B:THR:HG22  | 1        | 0.2           |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG22  | 1        | 0.2           |
| (1,597)  | 1:107:A:ALA:HB2  | 1:83:A:THR:HA    | 4        | 0.2           |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 16       | 0.2           |
| (1,416)  | 1:39:B:LEU:H     | 1:38:B:VAL:HG11  | 8        | 0.2           |
| (1,416)  | 1:39:B:LEU:H     | 1:38:B:VAL:HG13  | 17       | 0.2           |
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG13  | 6        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG11  | 8        | 0.2           |
| (1,415)  | 1:39:A:LEU:H     | 1:38:A:VAL:HG13  | 17       | 0.2           |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG23 | 8        | 0.2           |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG21 | 13       | 0.2           |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG23 | 8        | 0.2           |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG21 | 13       | 0.2           |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 1        | 0.2           |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 5        | 0.2           |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 6        | 0.2           |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 11       | 0.2           |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 13       | 0.2           |
| (1,396)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG13 | 18       | 0.2           |
| (1,396)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG13 | 20       | 0.2           |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 1        | 0.2           |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 5        | 0.2           |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 6        | 0.2           |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 11       | 0.2           |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 13       | 0.2           |
| (1,395)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG13 | 18       | 0.2           |
| (1,395)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG13 | 20       | 0.2           |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 4        | 0.2           |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 4        | 0.2           |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 14       | 0.2           |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE3   | 12       | 0.2           |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG21  | 6        | 0.2           |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG21  | 6        | 0.2           |
| (1,239)  | 1:20:A:VAL:HA    | 1:20:A:VAL:HG23  | 9        | 0.2           |
| (1,238)  | 1:55:B:GLU:H     | 1:20:B:VAL:HA    | 14       | 0.2           |
| (1,237)  | 1:55:A:GLU:H     | 1:20:A:VAL:HA    | 14       | 0.2           |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 9        | 0.2           |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 16       | 0.2           |
| (3,16)   | 1:28:B:ALA:H     | 1:103:B:ARG:H    | 5        | 0.19          |
| (3,15)   | 1:28:A:ALA:H     | 1:103:A:ARG:H    | 5        | 0.19          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 16       | 0.19          |
| (2,6)    | 1:18:B:VAL:HB    | 1:59:B:ARG:HG2   | 7        | 0.19          |
| (2,5)    | 1:18:A:VAL:HB    | 1:59:A:ARG:HG2   | 7        | 0.19          |
| (1,3091) | 1:86:A:PHE:H     | 1:54:B:PHE:HD1   | 20       | 0.19          |
| (1,3085) | 1:112:A:LEU:HD11 | 1:14:B:VAL:HG21  | 14       | 0.19          |
| (1,3079) | 1:11:A:GLU:HG2   | 1:111:B:VAL:HG23 | 2        | 0.19          |
| (1,3053) | 1:70:A:GLY:HA3   | 1:112:B:LEU:HG   | 16       | 0.19          |
| (1,3050) | 1:21:B:TRP:HH2   | 1:31:A:ILE:HD12  | 11       | 0.19          |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 19       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 19       | 0.19          |
| (1,2872) | 1:73:B:SER:H     | 1:71:B:ILE:HB    | 4        | 0.19          |
| (1,2871) | 1:73:A:SER:H     | 1:71:A:ILE:HB    | 4        | 0.19          |
| (1,2839) | 1:74:A:LYS:H     | 1:72:A:ASP:HA    | 7        | 0.19          |
| (1,2719) | 1:84:A:HIS:H     | 1:83:A:THR:HB    | 1        | 0.19          |
| (1,2686) | 1:104:B:ILE:H    | 1:84:B:HIS:HB3   | 17       | 0.19          |
| (1,2685) | 1:104:A:ILE:H    | 1:84:A:HIS:HB3   | 17       | 0.19          |
| (1,2666) | 1:34:B:LYS:H     | 1:34:B:LYS:HD3   | 8        | 0.19          |
| (1,2665) | 1:34:A:LYS:H     | 1:34:A:LYS:HD3   | 8        | 0.19          |
| (1,2580) | 1:107:B:ALA:H    | 1:82:B:THR:HG21  | 3        | 0.19          |
| (1,2579) | 1:107:A:ALA:H    | 1:82:A:THR:HG21  | 3        | 0.19          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 14       | 0.19          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 2        | 0.19          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 12       | 0.19          |
| (1,2254) | 1:77:B:ASN:HD22  | 1:114:B:ARG:HA   | 20       | 0.19          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 12       | 0.19          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 16       | 0.19          |
| (1,2084) | 1:88:B:LYS:H     | 1:88:B:LYS:HD2   | 19       | 0.19          |
| (1,2083) | 1:88:A:LYS:H     | 1:88:A:LYS:HD2   | 19       | 0.19          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 7        | 0.19          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 2        | 0.19          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 7        | 0.19          |
| (1,1910) | 1:72:B:ASP:H     | 1:71:B:ILE:HG23  | 7        | 0.19          |
| (1,1909) | 1:72:A:ASP:H     | 1:71:A:ILE:HG23  | 7        | 0.19          |
| (1,1898) | 1:48:B:VAL:H     | 1:48:B:VAL:HG12  | 11       | 0.19          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG22  | 9        | 0.19          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 12       | 0.19          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG21 | 18       | 0.19          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG21 | 18       | 0.19          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG23 | 4        | 0.19          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG22 | 5        | 0.19          |
| (1,1508) | 1:102:B:ILE:HG13 | 1:102:B:ILE:HG23 | 18       | 0.19          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG23 | 4        | 0.19          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG22 | 5        | 0.19          |
| (1,1507) | 1:102:A:ILE:HG13 | 1:102:A:ILE:HG23 | 18       | 0.19          |
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG21  | 2        | 0.19          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG23  | 9        | 0.19          |
| (1,1354) | 1:104:B:ILE:HD13 | 1:87:B:VAL:HG21  | 18       | 0.19          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG21  | 2        | 0.19          |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG23  | 9        | 0.19          |
| (1,1353) | 1:104:A:ILE:HD13 | 1:87:A:VAL:HG21  | 18       | 0.19          |
| (1,1348) | 1:87:B:VAL:HG12  | 1:104:B:ILE:HD12 | 15       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1347) | 1:87:A:VAL:HG12  | 1:104:A:ILE:HD12 | 15       | 0.19          |
| (1,1300) | 1:36:B:VAL:HG22  | 1:91:B:THR:HB    | 1        | 0.19          |
| (1,1299) | 1:36:A:VAL:HG22  | 1:91:A:THR:HB    | 1        | 0.19          |
| (1,988)  | 1:27:B:THR:HG21  | 1:35:B:GLU:HG3   | 6        | 0.19          |
| (1,854)  | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 1        | 0.19          |
| (1,854)  | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 3        | 0.19          |
| (1,853)  | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 1        | 0.19          |
| (1,853)  | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 3        | 0.19          |
| (1,806)  | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 20       | 0.19          |
| (1,805)  | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 20       | 0.19          |
| (1,598)  | 1:107:B:ALA:HB2  | 1:83:B:THR:HA    | 4        | 0.19          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 6        | 0.19          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 14       | 0.19          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 16       | 0.19          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 6        | 0.19          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 14       | 0.19          |
| (1,554)  | 1:88:B:LYS:HG2   | 1:88:B:LYS:HE2   | 19       | 0.19          |
| (1,553)  | 1:88:A:LYS:HG2   | 1:88:A:LYS:HE2   | 19       | 0.19          |
| (1,460)  | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12  | 1        | 0.19          |
| (1,459)  | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12  | 1        | 0.19          |
| (1,404)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG21 | 3        | 0.19          |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG22 | 11       | 0.19          |
| (1,403)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG21 | 3        | 0.19          |
| (1,396)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG13 | 3        | 0.19          |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 4        | 0.19          |
| (1,396)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG13 | 7        | 0.19          |
| (1,396)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG13 | 8        | 0.19          |
| (1,396)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG13 | 9        | 0.19          |
| (1,396)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG13 | 14       | 0.19          |
| (1,396)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG13 | 15       | 0.19          |
| (1,396)  | 1:102:B:ILE:HD13 | 1:102:B:ILE:HG13 | 16       | 0.19          |
| (1,395)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG13 | 3        | 0.19          |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 4        | 0.19          |
| (1,395)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG13 | 7        | 0.19          |
| (1,395)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG13 | 8        | 0.19          |
| (1,395)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG13 | 9        | 0.19          |
| (1,395)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG13 | 14       | 0.19          |
| (1,395)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG13 | 15       | 0.19          |
| (1,395)  | 1:102:A:ILE:HD13 | 1:102:A:ILE:HG13 | 16       | 0.19          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 8        | 0.19          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 14       | 0.19          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 19       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 8        | 0.19          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 19       | 0.19          |
| (1,281)  | 1:37:A:MET:HA    | 1:37:A:MET:HE3   | 12       | 0.19          |
| (1,272)  | 1:14:B:VAL:HG13  | 1:15:B:CYS:HB2   | 11       | 0.19          |
| (1,240)  | 1:20:B:VAL:HA    | 1:20:B:VAL:HG23  | 9        | 0.19          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 9        | 0.19          |
| (3,15)   | 1:28:A:ALA:H     | 1:35:A:GLU:H     | 20       | 0.18          |
| (1,3096) | 1:69:B:ARG:HA    | 1:112:A:LEU:HD22 | 4        | 0.18          |
| (1,3088) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HA    | 18       | 0.18          |
| (1,3086) | 1:112:B:LEU:HD11 | 1:14:A:VAL:HG21  | 14       | 0.18          |
| (1,3060) | 1:71:B:ILE:HD11  | 1:14:A:VAL:HB    | 17       | 0.18          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 14       | 0.18          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 4        | 0.18          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 6        | 0.18          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 4        | 0.18          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 6        | 0.18          |
| (1,2976) | 1:103:B:ARG:H    | 1:103:B:ARG:HG2  | 19       | 0.18          |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 17       | 0.18          |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 19       | 0.18          |
| (1,2702) | 1:104:B:ILE:H    | 1:103:B:ARG:HB3  | 9        | 0.18          |
| (1,2701) | 1:104:A:ILE:H    | 1:103:A:ARG:HB3  | 9        | 0.18          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB2   | 18       | 0.18          |
| (1,2387) | 1:29:A:THR:H     | 1:28:A:ALA:HB2   | 18       | 0.18          |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 12       | 0.18          |
| (1,2383) | 1:29:A:THR:H     | 1:30:A:ASP:HB2   | 2        | 0.18          |
| (1,2228) | 1:118:B:ARG:H    | 1:117:B:VAL:HA   | 9        | 0.18          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 9        | 0.18          |
| (1,2227) | 1:118:A:ARG:H    | 1:117:A:VAL:HA   | 12       | 0.18          |
| (1,2222) | 1:118:B:ARG:H    | 1:117:B:VAL:HB   | 8        | 0.18          |
| (1,2221) | 1:118:A:ARG:H    | 1:117:A:VAL:HB   | 8        | 0.18          |
| (1,2160) | 1:77:B:ASN:H     | 1:115:B:LYS:HG2  | 6        | 0.18          |
| (1,2159) | 1:77:A:ASN:H     | 1:115:A:LYS:HG2  | 6        | 0.18          |
| (1,2126) | 1:32:B:LYS:H     | 1:31:B:ILE:HG12  | 12       | 0.18          |
| (1,2125) | 1:32:A:LYS:H     | 1:31:A:ILE:HG12  | 12       | 0.18          |
| (1,2125) | 1:32:A:LYS:H     | 1:31:A:ILE:HG12  | 18       | 0.18          |
| (1,2046) | 1:27:B:THR:H     | 1:28:B:ALA:H     | 13       | 0.18          |
| (1,2045) | 1:27:A:THR:H     | 1:28:A:ALA:H     | 13       | 0.18          |
| (1,2014) | 1:79:B:TYR:H     | 1:111:B:VAL:HB   | 4        | 0.18          |
| (1,2013) | 1:79:A:TYR:H     | 1:111:A:VAL:HB   | 13       | 0.18          |
| (1,2002) | 1:79:B:TYR:H     | 1:111:B:VAL:HA   | 10       | 0.18          |
| (1,2001) | 1:79:A:TYR:H     | 1:111:A:VAL:HA   | 10       | 0.18          |
| (1,1914) | 1:72:B:ASP:H     | 1:71:B:ILE:HA    | 7        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1913) | 1:72:A:ASP:H     | 1:71:A:ILE:HA    | 7        | 0.18          |
| (1,1897) | 1:48:A:VAL:H     | 1:48:A:VAL:HG12  | 11       | 0.18          |
| (1,1768) | 1:20:B:VAL:H     | 1:20:B:VAL:HG23  | 9        | 0.18          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 12       | 0.18          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG23  | 3        | 0.18          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG23  | 3        | 0.18          |
| (1,1348) | 1:87:B:VAL:HG12  | 1:104:B:ILE:HD12 | 9        | 0.18          |
| (1,1172) | 1:39:B:LEU:HD21  | 1:92:B:MET:HG2   | 20       | 0.18          |
| (1,1171) | 1:39:A:LEU:HD21  | 1:92:A:MET:HG2   | 20       | 0.18          |
| (1,806)  | 1:118:B:ARG:HG3  | 1:118:B:ARG:HB2  | 12       | 0.18          |
| (1,805)  | 1:118:A:ARG:HG3  | 1:118:A:ARG:HB2  | 12       | 0.18          |
| (1,688)  | 1:55:B:GLU:H     | 1:20:B:VAL:HG23  | 6        | 0.18          |
| (1,687)  | 1:55:A:GLU:H     | 1:20:A:VAL:HG23  | 6        | 0.18          |
| (1,584)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HD2  | 11       | 0.18          |
| (1,583)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HD2  | 11       | 0.18          |
| (1,423)  | 1:87:A:VAL:HG11  | 1:53:A:PHE:HD1   | 11       | 0.18          |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG23 | 1        | 0.18          |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG23 | 1        | 0.18          |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG22 | 11       | 0.18          |
| (1,402)  | 1:102:B:ILE:HD11 | 1:25:B:LYS:HG2   | 4        | 0.18          |
| (1,401)  | 1:102:A:ILE:HD11 | 1:25:A:LYS:HG2   | 4        | 0.18          |
| (1,396)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG13 | 2        | 0.18          |
| (1,396)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG13 | 10       | 0.18          |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 17       | 0.18          |
| (1,396)  | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG13 | 19       | 0.18          |
| (1,395)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG13 | 2        | 0.18          |
| (1,395)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG13 | 10       | 0.18          |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 17       | 0.18          |
| (1,395)  | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG13 | 19       | 0.18          |
| (1,308)  | 1:71:B:ILE:HG23  | 1:76:B:TRP:HB3   | 8        | 0.18          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 6        | 0.18          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 16       | 0.18          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 6        | 0.18          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 16       | 0.18          |
| (1,282)  | 1:37:B:MET:HA    | 1:37:B:MET:HE1   | 13       | 0.18          |
| (1,281)  | 1:37:A:MET:HA    | 1:37:A:MET:HE1   | 13       | 0.18          |
| (1,271)  | 1:14:A:VAL:HG13  | 1:15:A:CYS:HB2   | 11       | 0.18          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 1        | 0.18          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 6        | 0.18          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 8        | 0.18          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 14       | 0.18          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 1        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,67)   | 1:32:A:LYS:HE2  | 1:32:A:LYS:HG3   | 8        | 0.18          |
| (1,67)   | 1:32:A:LYS:HE2  | 1:32:A:LYS:HG3   | 14       | 0.18          |
| (3,16)   | 1:28:B:ALA:H    | 1:35:B:GLU:H     | 20       | 0.17          |
| (1,3095) | 1:69:A:ARG:HA   | 1:112:B:LEU:HD22 | 4        | 0.17          |
| (1,3092) | 1:86:B:PHE:H    | 1:54:A:PHE:HD2   | 9        | 0.17          |
| (1,3091) | 1:86:A:PHE:H    | 1:54:B:PHE:HD2   | 9        | 0.17          |
| (1,3059) | 1:71:A:ILE:HD13 | 1:14:B:VAL:HB    | 18       | 0.17          |
| (1,3004) | 1:28:B:ALA:H    | 1:38:B:VAL:HG11  | 16       | 0.17          |
| (1,3003) | 1:28:A:ALA:H    | 1:38:A:VAL:HG13  | 14       | 0.17          |
| (1,3003) | 1:28:A:ALA:H    | 1:38:A:VAL:HG11  | 16       | 0.17          |
| (1,2976) | 1:103:B:ARG:H   | 1:103:B:ARG:HG2  | 5        | 0.17          |
| (1,2976) | 1:103:B:ARG:H   | 1:103:B:ARG:HG2  | 17       | 0.17          |
| (1,2975) | 1:103:A:ARG:H   | 1:103:A:ARG:HG2  | 5        | 0.17          |
| (1,2975) | 1:103:A:ARG:H   | 1:103:A:ARG:HG2  | 6        | 0.17          |
| (1,2906) | 1:22:B:VAL:H    | 1:53:B:PHE:HB3   | 16       | 0.17          |
| (1,2905) | 1:22:A:VAL:H    | 1:53:A:PHE:HB3   | 16       | 0.17          |
| (1,2764) | 1:18:B:VAL:H    | 1:108:B:CYS:HB3  | 4        | 0.17          |
| (1,2763) | 1:18:A:VAL:H    | 1:108:A:CYS:HB3  | 4        | 0.17          |
| (1,2720) | 1:84:B:HIS:H    | 1:83:B:THR:HB    | 16       | 0.17          |
| (1,2719) | 1:84:A:HIS:H    | 1:83:A:THR:HB    | 20       | 0.17          |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB2  | 4        | 0.17          |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB2  | 6        | 0.17          |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB1  | 18       | 0.17          |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB2  | 4        | 0.17          |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB2  | 6        | 0.17          |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB1  | 18       | 0.17          |
| (1,2503) | 1:30:A:ASP:H    | 1:34:A:LYS:HB2   | 4        | 0.17          |
| (1,2503) | 1:30:A:ASP:H    | 1:34:A:LYS:HB2   | 18       | 0.17          |
| (1,2196) | 1:55:B:GLU:H    | 1:22:B:VAL:HG12  | 15       | 0.17          |
| (1,2195) | 1:55:A:GLU:H    | 1:22:A:VAL:HG12  | 15       | 0.17          |
| (1,2170) | 1:46:B:ASN:HD21 | 1:46:B:ASN:HA    | 4        | 0.17          |
| (1,2167) | 1:46:A:ASN:HD21 | 1:45:A:ASN:HA    | 4        | 0.17          |
| (1,2126) | 1:32:B:LYS:H    | 1:31:B:ILE:HG12  | 18       | 0.17          |
| (1,2014) | 1:79:B:TYR:H    | 1:111:B:VAL:HB   | 1        | 0.17          |
| (1,2014) | 1:79:B:TYR:H    | 1:111:B:VAL:HB   | 13       | 0.17          |
| (1,2013) | 1:79:A:TYR:H    | 1:111:A:VAL:HB   | 1        | 0.17          |
| (1,2013) | 1:79:A:TYR:H    | 1:111:A:VAL:HB   | 4        | 0.17          |
| (1,1895) | 1:44:A:ILE:H    | 1:48:A:VAL:H     | 5        | 0.17          |
| (1,1767) | 1:20:A:VAL:H    | 1:20:A:VAL:HG23  | 9        | 0.17          |
| (1,1701) | 1:31:A:ILE:H    | 1:102:A:ILE:HG22 | 10       | 0.17          |
| (1,1649) | 1:47:A:SER:H    | 1:48:A:VAL:HG12  | 16       | 0.17          |
| (1,1361) | 1:104:A:ILE:HB  | 1:87:A:VAL:HG22  | 20       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1354) | 1:104:B:ILE:HD12 | 1:87:B:VAL:HG22  | 3        | 0.17          |
| (1,1353) | 1:104:A:ILE:HD12 | 1:87:A:VAL:HG22  | 3        | 0.17          |
| (1,1347) | 1:87:A:VAL:HG12  | 1:104:A:ILE:HD12 | 9        | 0.17          |
| (1,1208) | 1:37:B:MET:HB2   | 1:26:B:THR:HG21  | 15       | 0.17          |
| (1,1207) | 1:37:A:MET:HB2   | 1:26:A:THR:HG21  | 15       | 0.17          |
| (1,1187) | 1:31:A:ILE:HD13  | 1:101:A:PHE:HB2  | 8        | 0.17          |
| (1,1172) | 1:39:B:LEU:HD22  | 1:92:B:MET:HG2   | 6        | 0.17          |
| (1,1171) | 1:39:A:LEU:HD22  | 1:92:A:MET:HG2   | 6        | 0.17          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 17       | 0.17          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 17       | 0.17          |
| (1,960)  | 1:59:B:ARG:HD2   | 1:18:B:VAL:HB    | 18       | 0.17          |
| (1,959)  | 1:59:A:ARG:HD2   | 1:18:A:VAL:HB    | 18       | 0.17          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 11       | 0.17          |
| (1,424)  | 1:87:B:VAL:HG11  | 1:53:B:PHE:HD1   | 11       | 0.17          |
| (1,396)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG13 | 12       | 0.17          |
| (1,395)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG13 | 12       | 0.17          |
| (1,357)  | 1:41:A:GLU:H     | 1:41:A:GLU:HG2   | 19       | 0.17          |
| (1,344)  | 1:48:B:VAL:HG12  | 1:41:B:GLU:HG2   | 3        | 0.17          |
| (1,343)  | 1:48:A:VAL:HG12  | 1:41:A:GLU:HG2   | 3        | 0.17          |
| (1,307)  | 1:71:A:ILE:HG23  | 1:76:A:TRP:HB3   | 8        | 0.17          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 7        | 0.17          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 7        | 0.17          |
| (1,294)  | 1:106:B:THR:HG22 | 1:85:B:THR:HB    | 1        | 0.17          |
| (1,293)  | 1:106:A:THR:HG22 | 1:85:A:THR:HB    | 1        | 0.17          |
| (1,250)  | 1:112:B:LEU:HD23 | 1:76:B:TRP:HD1   | 5        | 0.17          |
| (1,249)  | 1:112:A:LEU:HD23 | 1:76:A:TRP:HD1   | 5        | 0.17          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 7        | 0.17          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 5        | 0.17          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 7        | 0.17          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 15       | 0.17          |
| (1,60)   | 1:42:B:VAL:HG21  | 1:49:B:PHE:HA    | 9        | 0.17          |
| (1,59)   | 1:42:A:VAL:HG21  | 1:49:A:PHE:HA    | 9        | 0.17          |
| (1,3091) | 1:86:A:PHE:H     | 1:54:B:PHE:HD2   | 18       | 0.16          |
| (1,3067) | 1:70:A:GLY:HA3   | 1:71:B:ILE:HG23  | 12       | 0.16          |
| (1,3059) | 1:71:A:ILE:HD11  | 1:14:B:VAL:HB    | 17       | 0.16          |
| (1,3054) | 1:70:B:GLY:HA3   | 1:112:A:LEU:HG   | 16       | 0.16          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 11       | 0.16          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 15       | 0.16          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 15       | 0.16          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG13  | 14       | 0.16          |
| (1,2976) | 1:103:B:ARG:H    | 1:103:B:ARG:HG2  | 6        | 0.16          |
| (1,2854) | 1:73:B:SER:H     | 1:76:B:TRP:HB3   | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2853) | 1:73:A:SER:H    | 1:76:A:TRP:HB3   | 13       | 0.16          |
| (1,2764) | 1:18:B:VAL:H    | 1:108:B:CYS:HB3  | 2        | 0.16          |
| (1,2763) | 1:18:A:VAL:H    | 1:108:A:CYS:HB3  | 2        | 0.16          |
| (1,2720) | 1:84:B:HIS:H    | 1:83:B:THR:HB    | 20       | 0.16          |
| (1,2719) | 1:84:A:HIS:H    | 1:83:A:THR:HB    | 16       | 0.16          |
| (1,2620) | 1:19:B:SER:H    | 1:20:B:VAL:HG22  | 14       | 0.16          |
| (1,2619) | 1:19:A:SER:H    | 1:20:A:VAL:HG22  | 14       | 0.16          |
| (1,2597) | 1:107:A:ALA:H   | 1:108:A:CYS:HB3  | 15       | 0.16          |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB3  | 17       | 0.16          |
| (1,2587) | 1:107:A:ALA:H   | 1:107:A:ALA:HB3  | 17       | 0.16          |
| (1,2504) | 1:30:B:ASP:H    | 1:34:B:LYS:HB2   | 4        | 0.16          |
| (1,2504) | 1:30:B:ASP:H    | 1:34:B:LYS:HB2   | 9        | 0.16          |
| (1,2504) | 1:30:B:ASP:H    | 1:34:B:LYS:HB2   | 15       | 0.16          |
| (1,2504) | 1:30:B:ASP:H    | 1:34:B:LYS:HB2   | 18       | 0.16          |
| (1,2503) | 1:30:A:ASP:H    | 1:34:A:LYS:HB2   | 9        | 0.16          |
| (1,2503) | 1:30:A:ASP:H    | 1:34:A:LYS:HB2   | 15       | 0.16          |
| (1,2390) | 1:29:B:THR:H    | 1:102:B:ILE:HG21 | 20       | 0.16          |
| (1,2389) | 1:29:A:THR:H    | 1:102:A:ILE:HG21 | 20       | 0.16          |
| (1,2387) | 1:29:A:THR:H    | 1:28:A:ALA:HB2   | 3        | 0.16          |
| (1,2227) | 1:118:A:ARG:H   | 1:117:A:VAL:HA   | 19       | 0.16          |
| (1,2169) | 1:46:A:ASN:HD21 | 1:46:A:ASN:HA    | 4        | 0.16          |
| (1,2168) | 1:46:B:ASN:HD21 | 1:45:B:ASN:HA    | 4        | 0.16          |
| (1,2084) | 1:88:B:LYS:H    | 1:88:B:LYS:HD2   | 3        | 0.16          |
| (1,2083) | 1:88:A:LYS:H    | 1:88:A:LYS:HD2   | 3        | 0.16          |
| (1,2046) | 1:27:B:THR:H    | 1:28:B:ALA:H     | 8        | 0.16          |
| (1,2046) | 1:27:B:THR:H    | 1:28:B:ALA:H     | 17       | 0.16          |
| (1,2045) | 1:27:A:THR:H    | 1:28:A:ALA:H     | 8        | 0.16          |
| (1,2045) | 1:27:A:THR:H    | 1:28:A:ALA:H     | 17       | 0.16          |
| (1,1925) | 1:72:A:ASP:H    | 1:71:A:ILE:HD12  | 10       | 0.16          |
| (1,1897) | 1:48:A:VAL:H    | 1:48:A:VAL:HG12  | 6        | 0.16          |
| (1,1896) | 1:44:B:ILE:H    | 1:48:B:VAL:H     | 5        | 0.16          |
| (1,1880) | 1:21:B:TRP:H    | 1:20:B:VAL:HG22  | 19       | 0.16          |
| (1,1702) | 1:31:B:ILE:H    | 1:102:B:ILE:HG22 | 8        | 0.16          |
| (1,1702) | 1:31:B:ILE:H    | 1:102:B:ILE:HG22 | 10       | 0.16          |
| (1,1701) | 1:31:A:ILE:H    | 1:102:A:ILE:HG22 | 8        | 0.16          |
| (1,1625) | 1:113:A:SER:H   | 1:76:A:TRP:HB2   | 19       | 0.16          |
| (1,1384) | 1:18:B:VAL:HG21 | 1:59:B:ARG:HG2   | 13       | 0.16          |
| (1,1362) | 1:104:B:ILE:HB  | 1:87:B:VAL:HG22  | 20       | 0.16          |
| (1,1361) | 1:104:A:ILE:HB  | 1:87:A:VAL:HG21  | 4        | 0.16          |
| (1,1348) | 1:87:B:VAL:HG11 | 1:104:B:ILE:HD12 | 14       | 0.16          |
| (1,1347) | 1:87:A:VAL:HG11 | 1:104:A:ILE:HD12 | 14       | 0.16          |
| (1,1188) | 1:31:B:ILE:HD13 | 1:101:B:PHE:HB2  | 8        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG21  | 2        | 0.16          |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG22  | 5        | 0.16          |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG21  | 11       | 0.16          |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG22  | 14       | 0.16          |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG22  | 16       | 0.16          |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG22  | 17       | 0.16          |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG23  | 18       | 0.16          |
| (1,1002) | 1:22:B:VAL:HB    | 1:22:B:VAL:HG21  | 20       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG21  | 2        | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG23  | 4        | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG23  | 7        | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG23  | 10       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG21  | 11       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG22  | 14       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG22  | 16       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG22  | 17       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG23  | 18       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG21  | 19       | 0.16          |
| (1,1001) | 1:22:A:VAL:HB    | 1:22:A:VAL:HG21  | 20       | 0.16          |
| (1,905)  | 1:9:A:ARG:H      | 1:9:A:ARG:HB2    | 8        | 0.16          |
| (1,712)  | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 20       | 0.16          |
| (1,711)  | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 20       | 0.16          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 11       | 0.16          |
| (1,426)  | 1:87:B:VAL:HG11  | 1:53:B:PHE:HE1   | 16       | 0.16          |
| (1,358)  | 1:41:B:GLU:H     | 1:41:B:GLU:HG2   | 19       | 0.16          |
| (1,344)  | 1:48:B:VAL:HG11  | 1:41:B:GLU:HG2   | 10       | 0.16          |
| (1,343)  | 1:48:A:VAL:HG11  | 1:41:A:GLU:HG2   | 10       | 0.16          |
| (1,300)  | 1:50:B:LYS:HD2   | 1:50:B:LYS:HG3   | 15       | 0.16          |
| (1,299)  | 1:50:A:LYS:HD2   | 1:50:A:LYS:HG3   | 15       | 0.16          |
| (1,250)  | 1:112:B:LEU:HD22 | 1:76:B:TRP:HD1   | 1        | 0.16          |
| (1,249)  | 1:112:A:LEU:HD22 | 1:76:A:TRP:HD1   | 1        | 0.16          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 5        | 0.16          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 15       | 0.16          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 6        | 0.16          |
| (1,3094) | 1:86:B:PHE:H     | 1:54:A:PHE:HE1   | 3        | 0.15          |
| (1,3068) | 1:70:B:GLY:HA3   | 1:71:A:ILE:HG23  | 12       | 0.15          |
| (1,3056) | 1:107:B:ALA:HB1  | 1:109:A:VAL:HG11 | 14       | 0.15          |
| (1,3014) | 1:28:B:ALA:H     | 1:29:B:THR:HA    | 18       | 0.15          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 11       | 0.15          |
| (1,3013) | 1:28:A:ALA:H     | 1:29:A:THR:HA    | 18       | 0.15          |
| (1,2720) | 1:84:B:HIS:H     | 1:83:B:THR:HB    | 19       | 0.15          |
| (1,2719) | 1:84:A:HIS:H     | 1:83:A:THR:HB    | 19       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2598) | 1:107:B:ALA:H   | 1:108:B:CYS:HB3  | 15       | 0.15          |
| (1,2392) | 1:29:B:THR:H    | 1:103:B:ARG:H    | 11       | 0.15          |
| (1,2391) | 1:29:A:THR:H    | 1:103:A:ARG:H    | 11       | 0.15          |
| (1,2390) | 1:29:B:THR:H    | 1:102:B:ILE:HG22 | 8        | 0.15          |
| (1,2388) | 1:29:B:THR:H    | 1:28:B:ALA:HB2   | 3        | 0.15          |
| (1,2384) | 1:29:B:THR:H    | 1:30:B:ASP:HB2   | 6        | 0.15          |
| (1,2383) | 1:29:A:THR:H    | 1:30:A:ASP:HB2   | 6        | 0.15          |
| (1,2374) | 1:29:B:THR:H    | 1:102:B:ILE:HD13 | 5        | 0.15          |
| (1,2228) | 1:118:B:ARG:H   | 1:117:B:VAL:HA   | 19       | 0.15          |
| (1,2152) | 1:77:B:ASN:H    | 1:115:B:LYS:HD2  | 18       | 0.15          |
| (1,2014) | 1:79:B:TYR:H    | 1:111:B:VAL:HB   | 14       | 0.15          |
| (1,2013) | 1:79:A:TYR:H    | 1:111:A:VAL:HB   | 7        | 0.15          |
| (1,2013) | 1:79:A:TYR:H    | 1:111:A:VAL:HB   | 14       | 0.15          |
| (1,1928) | 1:72:B:ASP:H    | 1:71:B:ILE:HB    | 15       | 0.15          |
| (1,1927) | 1:72:A:ASP:H    | 1:71:A:ILE:HB    | 15       | 0.15          |
| (1,1926) | 1:72:B:ASP:H    | 1:71:B:ILE:HD12  | 10       | 0.15          |
| (1,1898) | 1:48:B:VAL:H    | 1:48:B:VAL:HG12  | 6        | 0.15          |
| (1,1879) | 1:21:A:TRP:H    | 1:20:A:VAL:HG22  | 19       | 0.15          |
| (1,1740) | 1:36:B:VAL:H    | 1:27:B:THR:HG23  | 4        | 0.15          |
| (1,1739) | 1:36:A:VAL:H    | 1:27:A:THR:HG23  | 4        | 0.15          |
| (1,1649) | 1:47:A:SER:H    | 1:48:A:VAL:HG11  | 13       | 0.15          |
| (1,1626) | 1:113:B:SER:H   | 1:76:B:TRP:HB2   | 19       | 0.15          |
| (1,1383) | 1:18:A:VAL:HG21 | 1:59:A:ARG:HG2   | 13       | 0.15          |
| (1,1362) | 1:104:B:ILE:HB  | 1:87:B:VAL:HG21  | 4        | 0.15          |
| (1,1348) | 1:87:B:VAL:HG12 | 1:104:B:ILE:HD11 | 4        | 0.15          |
| (1,1348) | 1:87:B:VAL:HG11 | 1:104:B:ILE:HD11 | 16       | 0.15          |
| (1,1347) | 1:87:A:VAL:HG12 | 1:104:A:ILE:HD11 | 4        | 0.15          |
| (1,1332) | 1:64:B:VAL:HG21 | 1:65:B:ASP:HB3   | 9        | 0.15          |
| (1,1331) | 1:64:A:VAL:HG21 | 1:65:A:ASP:HB3   | 9        | 0.15          |
| (1,1331) | 1:64:A:VAL:HG23 | 1:65:A:ASP:HB3   | 10       | 0.15          |
| (1,1314) | 1:70:B:GLY:H    | 1:64:B:VAL:HG12  | 5        | 0.15          |
| (1,1313) | 1:70:A:GLY:H    | 1:64:A:VAL:HG12  | 5        | 0.15          |
| (1,1298) | 1:36:B:VAL:HG22 | 1:91:B:THR:H     | 16       | 0.15          |
| (1,1297) | 1:36:A:VAL:HG22 | 1:91:A:THR:H     | 16       | 0.15          |
| (1,1266) | 1:70:B:GLY:HA2  | 1:71:B:ILE:HD11  | 6        | 0.15          |
| (1,1265) | 1:70:A:GLY:HA2  | 1:71:A:ILE:HD11  | 6        | 0.15          |
| (1,1252) | 1:68:B:CYS:HB3  | 1:14:B:VAL:HB    | 1        | 0.15          |
| (1,1251) | 1:68:A:CYS:HB3  | 1:14:A:VAL:HB    | 1        | 0.15          |
| (1,1248) | 1:71:B:ILE:HG12 | 1:70:B:GLY:HA3   | 19       | 0.15          |
| (1,1002) | 1:22:B:VAL:HB   | 1:22:B:VAL:HG22  | 1        | 0.15          |
| (1,1002) | 1:22:B:VAL:HB   | 1:22:B:VAL:HG21  | 3        | 0.15          |
| (1,1002) | 1:22:B:VAL:HB   | 1:22:B:VAL:HG23  | 4        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG22 | 6        | 0.15          |
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG23 | 7        | 0.15          |
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG21 | 8        | 0.15          |
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG23 | 10       | 0.15          |
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG21 | 12       | 0.15          |
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG22 | 13       | 0.15          |
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG21 | 15       | 0.15          |
| (1,1002) | 1:22:B:VAL:HB  | 1:22:B:VAL:HG21 | 19       | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG22 | 1        | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG21 | 3        | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG22 | 5        | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG22 | 6        | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG21 | 8        | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG21 | 12       | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG22 | 13       | 0.15          |
| (1,1001) | 1:22:A:VAL:HB  | 1:22:A:VAL:HG21 | 15       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 1        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 2        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 3        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 4        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 5        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 6        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 7        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 8        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 9        | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 10       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 11       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 12       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 13       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 14       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 15       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 16       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 17       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 18       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 19       | 0.15          |
| (1,968)  | 1:32:B:LYS:HG3 | 1:32:B:LYS:HG2  | 20       | 0.15          |
| (1,967)  | 1:32:A:LYS:HG3 | 1:32:A:LYS:HG2  | 1        | 0.15          |
| (1,967)  | 1:32:A:LYS:HG3 | 1:32:A:LYS:HG2  | 2        | 0.15          |
| (1,967)  | 1:32:A:LYS:HG3 | 1:32:A:LYS:HG2  | 3        | 0.15          |
| (1,967)  | 1:32:A:LYS:HG3 | 1:32:A:LYS:HG2  | 4        | 0.15          |
| (1,967)  | 1:32:A:LYS:HG3 | 1:32:A:LYS:HG2  | 5        | 0.15          |
| (1,967)  | 1:32:A:LYS:HG3 | 1:32:A:LYS:HG2  | 6        | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 7        | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 8        | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 9        | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 10       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 11       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 12       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 13       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 14       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 15       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 16       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 17       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 18       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 19       | 0.15          |
| (1,967) | 1:32:A:LYS:HG3   | 1:32:A:LYS:HG2   | 20       | 0.15          |
| (1,912) | 1:9:B:ARG:HB2    | 1:6:B:ILE:HG13   | 4        | 0.15          |
| (1,911) | 1:9:A:ARG:HB2    | 1:6:A:ILE:HG13   | 4        | 0.15          |
| (1,906) | 1:9:B:ARG:H      | 1:9:B:ARG:HB2    | 8        | 0.15          |
| (1,906) | 1:9:B:ARG:H      | 1:9:B:ARG:HB2    | 14       | 0.15          |
| (1,905) | 1:9:A:ARG:H      | 1:9:A:ARG:HB2    | 14       | 0.15          |
| (1,854) | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 5        | 0.15          |
| (1,854) | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 9        | 0.15          |
| (1,853) | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 5        | 0.15          |
| (1,853) | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 9        | 0.15          |
| (1,712) | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 7        | 0.15          |
| (1,712) | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 9        | 0.15          |
| (1,712) | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 13       | 0.15          |
| (1,711) | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 7        | 0.15          |
| (1,711) | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 9        | 0.15          |
| (1,711) | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 13       | 0.15          |
| (1,596) | 1:107:B:ALA:HB2  | 1:106:B:THR:HA   | 16       | 0.15          |
| (1,595) | 1:107:A:ALA:HB2  | 1:106:A:THR:HA   | 16       | 0.15          |
| (1,538) | 1:115:B:LYS:HB2  | 1:115:B:LYS:HG2  | 12       | 0.15          |
| (1,538) | 1:115:B:LYS:HB2  | 1:115:B:LYS:HG2  | 13       | 0.15          |
| (1,537) | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 10       | 0.15          |
| (1,537) | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 12       | 0.15          |
| (1,537) | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 13       | 0.15          |
| (1,425) | 1:87:A:VAL:HG11  | 1:53:A:PHE:HE1   | 16       | 0.15          |
| (1,416) | 1:39:B:LEU:H     | 1:38:B:VAL:HG12  | 4        | 0.15          |
| (1,415) | 1:39:A:LEU:H     | 1:38:A:VAL:HG12  | 4        | 0.15          |
| (1,404) | 1:102:B:ILE:HD11 | 1:102:B:ILE:HG22 | 20       | 0.15          |
| (1,403) | 1:102:A:ILE:HD11 | 1:102:A:ILE:HG22 | 20       | 0.15          |
| (1,402) | 1:102:B:ILE:HD13 | 1:25:B:LYS:HG2   | 13       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,401)  | 1:102:A:ILE:HD13 | 1:25:A:LYS:HG2   | 13       | 0.15          |
| (1,340)  | 1:28:B:ALA:H     | 1:36:B:VAL:HG12  | 12       | 0.15          |
| (1,339)  | 1:28:A:ALA:H     | 1:36:A:VAL:HG12  | 12       | 0.15          |
| (1,68)   | 1:32:B:LYS:HE2   | 1:32:B:LYS:HG3   | 17       | 0.15          |
| (1,48)   | 1:42:B:VAL:HG21  | 1:44:B:ILE:HB    | 4        | 0.15          |
| (1,48)   | 1:42:B:VAL:HG21  | 1:44:B:ILE:HB    | 13       | 0.15          |
| (1,47)   | 1:42:A:VAL:HG21  | 1:44:A:ILE:HB    | 4        | 0.15          |
| (1,47)   | 1:42:A:VAL:HG21  | 1:44:A:ILE:HB    | 13       | 0.15          |
| (3,8)    | 1:79:B:TYR:H     | 1:71:B:ILE:HD11  | 5        | 0.14          |
| (3,7)    | 1:79:A:TYR:H     | 1:71:A:ILE:HD11  | 5        | 0.14          |
| (1,3092) | 1:86:B:PHE:H     | 1:54:A:PHE:HD2   | 18       | 0.14          |
| (1,3092) | 1:86:B:PHE:H     | 1:54:A:PHE:HD1   | 20       | 0.14          |
| (1,3069) | 1:11:A:GLU:H     | 1:113:B:SER:HB2  | 13       | 0.14          |
| (1,3020) | 1:28:B:ALA:H     | 1:28:B:ALA:HB3   | 18       | 0.14          |
| (1,3019) | 1:28:A:ALA:H     | 1:28:A:ALA:HB3   | 18       | 0.14          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG12  | 7        | 0.14          |
| (1,2976) | 1:103:B:ARG:H    | 1:103:B:ARG:HG2  | 1        | 0.14          |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 1        | 0.14          |
| (1,2665) | 1:34:A:LYS:H     | 1:34:A:LYS:HD3   | 2        | 0.14          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB2  | 7        | 0.14          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB2  | 7        | 0.14          |
| (1,2389) | 1:29:A:THR:H     | 1:102:A:ILE:HG22 | 8        | 0.14          |
| (1,2373) | 1:29:A:THR:H     | 1:102:A:ILE:HD13 | 5        | 0.14          |
| (1,2255) | 1:77:A:ASN:HD22  | 1:115:A:LYS:HG2  | 17       | 0.14          |
| (1,2151) | 1:77:A:ASN:H     | 1:115:A:LYS:HD2  | 18       | 0.14          |
| (1,2035) | 1:27:A:THR:H     | 1:38:A:VAL:HB    | 9        | 0.14          |
| (1,2032) | 1:27:B:THR:H     | 1:38:B:VAL:HG21  | 4        | 0.14          |
| (1,2031) | 1:27:A:THR:H     | 1:38:A:VAL:HG21  | 4        | 0.14          |
| (1,2014) | 1:79:B:TYR:H     | 1:111:B:VAL:HB   | 7        | 0.14          |
| (1,1905) | 1:48:A:VAL:H     | 1:48:A:VAL:HB    | 7        | 0.14          |
| (1,1898) | 1:48:B:VAL:H     | 1:48:B:VAL:HG11  | 15       | 0.14          |
| (1,1882) | 1:21:B:TRP:H     | 1:21:B:TRP:HZ2   | 16       | 0.14          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG21  | 13       | 0.14          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 11       | 0.14          |
| (1,1718) | 1:76:B:TRP:H     | 1:74:B:LYS:HD2   | 1        | 0.14          |
| (1,1717) | 1:76:A:TRP:H     | 1:74:A:LYS:HD2   | 1        | 0.14          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG23 | 2        | 0.14          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG11  | 13       | 0.14          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG12  | 16       | 0.14          |
| (1,1486) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HG21  | 7        | 0.14          |
| (1,1485) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HG21  | 7        | 0.14          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1449) | 1:25:A:LYS:HG2  | 1:53:A:PHE:HE1   | 19       | 0.14          |
| (1,1348) | 1:87:B:VAL:HG12 | 1:104:B:ILE:HD11 | 8        | 0.14          |
| (1,1347) | 1:87:A:VAL:HG12 | 1:104:A:ILE:HD11 | 8        | 0.14          |
| (1,1347) | 1:87:A:VAL:HG11 | 1:104:A:ILE:HD11 | 16       | 0.14          |
| (1,1332) | 1:64:B:VAL:HG23 | 1:65:B:ASP:HB3   | 10       | 0.14          |
| (1,1247) | 1:71:A:ILE:HG12 | 1:70:A:GLY:HA3   | 19       | 0.14          |
| (1,1088) | 1:115:B:LYS:HG2 | 1:114:B:ARG:HA   | 7        | 0.14          |
| (1,1087) | 1:115:A:LYS:HG2 | 1:114:A:ARG:HA   | 7        | 0.14          |
| (1,1064) | 1:57:B:LYS:HD2  | 1:57:B:LYS:HB2   | 3        | 0.14          |
| (1,1063) | 1:57:A:LYS:HD2  | 1:57:A:LYS:HB2   | 3        | 0.14          |
| (1,1002) | 1:22:B:VAL:HB   | 1:22:B:VAL:HG21  | 9        | 0.14          |
| (1,1001) | 1:22:A:VAL:HB   | 1:22:A:VAL:HG21  | 9        | 0.14          |
| (1,987)  | 1:27:A:THR:HG21 | 1:35:A:GLU:HG3   | 1        | 0.14          |
| (1,854)  | 1:37:B:MET:HG3  | 1:36:B:VAL:HA    | 16       | 0.14          |
| (1,853)  | 1:37:A:MET:HG3  | 1:36:A:VAL:HA    | 16       | 0.14          |
| (1,660)  | 1:51:B:GLN:H    | 1:42:B:VAL:HG13  | 16       | 0.14          |
| (1,659)  | 1:51:A:GLN:H    | 1:42:A:VAL:HG13  | 16       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 1        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 3        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 4        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 5        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 6        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 7        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 8        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 9        | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 10       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 11       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 14       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 15       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 16       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 17       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 18       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 19       | 0.14          |
| (1,538)  | 1:115:B:LYS:HB2 | 1:115:B:LYS:HG2  | 20       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 1        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 2        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 3        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 4        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 5        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 6        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 7        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2 | 1:115:A:LYS:HG2  | 8        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 9        | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 11       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 14       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 15       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 16       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 17       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 18       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 19       | 0.14          |
| (1,537)  | 1:115:A:LYS:HB2  | 1:115:A:LYS:HG2  | 20       | 0.14          |
| (1,404)  | 1:102:B:ILE:HD12 | 1:102:B:ILE:HG23 | 4        | 0.14          |
| (1,403)  | 1:102:A:ILE:HD12 | 1:102:A:ILE:HG23 | 4        | 0.14          |
| (1,334)  | 1:36:B:VAL:HG11  | 1:36:B:VAL:HB    | 7        | 0.14          |
| (1,333)  | 1:36:A:VAL:HG11  | 1:36:A:VAL:HB    | 7        | 0.14          |
| (1,67)   | 1:32:A:LYS:HE2   | 1:32:A:LYS:HG3   | 17       | 0.14          |
| (1,60)   | 1:42:B:VAL:HG23  | 1:49:B:PHE:HA    | 5        | 0.14          |
| (1,59)   | 1:42:A:VAL:HG23  | 1:49:A:PHE:HA    | 5        | 0.14          |
| (1,5)    | 1:79:A:TYR:H     | 1:111:A:VAL:HG21 | 11       | 0.14          |
| (1,3102) | 1:9:B:ARG:HB3    | 1:115:A:LYS:HA   | 4        | 0.13          |
| (1,3093) | 1:86:A:PHE:H     | 1:54:B:PHE:HE1   | 3        | 0.13          |
| (1,3091) | 1:86:A:PHE:H     | 1:54:B:PHE:HD1   | 5        | 0.13          |
| (1,3060) | 1:71:B:ILE:HD13  | 1:14:A:VAL:HB    | 18       | 0.13          |
| (1,3004) | 1:28:B:ALA:H     | 1:38:B:VAL:HG11  | 15       | 0.13          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG12  | 7        | 0.13          |
| (1,3003) | 1:28:A:ALA:H     | 1:38:A:VAL:HG11  | 15       | 0.13          |
| (1,2868) | 1:73:B:SER:H     | 1:71:B:ILE:HD11  | 4        | 0.13          |
| (1,2867) | 1:73:A:SER:H     | 1:71:A:ILE:HD11  | 4        | 0.13          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 6        | 0.13          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 7        | 0.13          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 8        | 0.13          |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 11       | 0.13          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 6        | 0.13          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 7        | 0.13          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 8        | 0.13          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 10       | 0.13          |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 11       | 0.13          |
| (1,2666) | 1:34:B:LYS:H     | 1:34:B:LYS:HD3   | 2        | 0.13          |
| (1,2614) | 1:19:B:SER:H     | 1:18:B:VAL:HG21  | 4        | 0.13          |
| (1,2613) | 1:19:A:SER:H     | 1:18:A:VAL:HG21  | 4        | 0.13          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB1  | 11       | 0.13          |
| (1,2588) | 1:107:B:ALA:H    | 1:107:B:ALA:HB3  | 12       | 0.13          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB1  | 11       | 0.13          |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB3  | 12       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2504) | 1:30:B:ASP:H     | 1:34:B:LYS:HB2   | 13       | 0.13          |
| (1,2388) | 1:29:B:THR:H     | 1:28:B:ALA:HB3   | 13       | 0.13          |
| (1,2256) | 1:77:B:ASN:HD22  | 1:115:B:LYS:HG2  | 17       | 0.13          |
| (1,2224) | 1:118:B:ARG:H    | 1:118:B:ARG:HB2  | 4        | 0.13          |
| (1,2223) | 1:118:A:ARG:H    | 1:118:A:ARG:HB2  | 4        | 0.13          |
| (1,2112) | 1:117:B:VAL:H    | 1:116:B:ALA:HB1  | 14       | 0.13          |
| (1,2084) | 1:88:B:LYS:H     | 1:88:B:LYS:HD2   | 13       | 0.13          |
| (1,2083) | 1:88:A:LYS:H     | 1:88:A:LYS:HD2   | 13       | 0.13          |
| (1,2036) | 1:27:B:THR:H     | 1:38:B:VAL:HB    | 9        | 0.13          |
| (1,2032) | 1:27:B:THR:H     | 1:38:B:VAL:HG22  | 17       | 0.13          |
| (1,1912) | 1:72:B:ASP:H     | 1:76:B:TRP:HB3   | 15       | 0.13          |
| (1,1911) | 1:72:A:ASP:H     | 1:76:A:TRP:HB3   | 15       | 0.13          |
| (1,1906) | 1:48:B:VAL:H     | 1:48:B:VAL:HB    | 7        | 0.13          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 7        | 0.13          |
| (1,1721) | 1:76:A:TRP:H     | 1:115:A:LYS:HG2  | 7        | 0.13          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG23 | 2        | 0.13          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG12  | 5        | 0.13          |
| (1,1640) | 1:13:B:SER:H     | 1:12:B:PHE:HB2   | 15       | 0.13          |
| (1,1639) | 1:13:A:SER:H     | 1:12:A:PHE:HB2   | 15       | 0.13          |
| (1,1610) | 1:24:B:ASP:H     | 1:22:B:VAL:HG21  | 12       | 0.13          |
| (1,1556) | 1:49:B:PHE:HA    | 1:48:B:VAL:HB    | 6        | 0.13          |
| (1,1555) | 1:49:A:PHE:HA    | 1:48:A:VAL:HB    | 6        | 0.13          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG12  | 16       | 0.13          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG12  | 16       | 0.13          |
| (1,1348) | 1:87:B:VAL:HG11  | 1:104:B:ILE:HD11 | 13       | 0.13          |
| (1,1347) | 1:87:A:VAL:HG12  | 1:104:A:ILE:HD11 | 10       | 0.13          |
| (1,1347) | 1:87:A:VAL:HG11  | 1:104:A:ILE:HD11 | 13       | 0.13          |
| (1,988)  | 1:27:B:THR:HG21  | 1:35:B:GLU:HG3   | 1        | 0.13          |
| (1,810)  | 1:118:B:ARG:HB2  | 1:118:B:ARG:HG2  | 12       | 0.13          |
| (1,809)  | 1:118:A:ARG:HB2  | 1:118:A:ARG:HG2  | 12       | 0.13          |
| (1,712)  | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 17       | 0.13          |
| (1,711)  | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 10       | 0.13          |
| (1,711)  | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 17       | 0.13          |
| (1,682)  | 1:22:B:VAL:HB    | 1:53:B:PHE:HD1   | 16       | 0.13          |
| (1,681)  | 1:22:A:VAL:HB    | 1:53:A:PHE:HD1   | 16       | 0.13          |
| (1,604)  | 1:104:B:ILE:HB   | 1:85:B:THR:HG21  | 13       | 0.13          |
| (1,603)  | 1:104:A:ILE:HB   | 1:85:A:THR:HG21  | 13       | 0.13          |
| (1,593)  | 1:108:A:CYS:H    | 1:107:A:ALA:HB2  | 3        | 0.13          |
| (1,538)  | 1:115:B:LYS:HB2  | 1:115:B:LYS:HG2  | 2        | 0.13          |
| (1,400)  | 1:102:B:ILE:HD13 | 1:87:B:VAL:HG22  | 18       | 0.13          |
| (1,399)  | 1:102:A:ILE:HD13 | 1:87:A:VAL:HG22  | 18       | 0.13          |
| (1,343)  | 1:48:A:VAL:HG11  | 1:41:A:GLU:HG2   | 6        | 0.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,334) | 1:36:B:VAL:HG13 | 1:36:B:VAL:HB  | 4        | 0.13          |
| (1,334) | 1:36:B:VAL:HG13 | 1:36:B:VAL:HB  | 11       | 0.13          |
| (1,334) | 1:36:B:VAL:HG11 | 1:36:B:VAL:HB  | 16       | 0.13          |
| (1,334) | 1:36:B:VAL:HG12 | 1:36:B:VAL:HB  | 17       | 0.13          |
| (1,334) | 1:36:B:VAL:HG13 | 1:36:B:VAL:HB  | 18       | 0.13          |
| (1,334) | 1:36:B:VAL:HG12 | 1:36:B:VAL:HB  | 20       | 0.13          |
| (1,333) | 1:36:A:VAL:HG13 | 1:36:A:VAL:HB  | 4        | 0.13          |
| (1,333) | 1:36:A:VAL:HG13 | 1:36:A:VAL:HB  | 11       | 0.13          |
| (1,333) | 1:36:A:VAL:HG11 | 1:36:A:VAL:HB  | 16       | 0.13          |
| (1,333) | 1:36:A:VAL:HG12 | 1:36:A:VAL:HB  | 17       | 0.13          |
| (1,333) | 1:36:A:VAL:HG13 | 1:36:A:VAL:HB  | 18       | 0.13          |
| (1,333) | 1:36:A:VAL:HG12 | 1:36:A:VAL:HB  | 20       | 0.13          |
| (1,280) | 1:88:B:LYS:HB2  | 1:88:B:LYS:HD2 | 12       | 0.13          |
| (1,279) | 1:88:A:LYS:HB2  | 1:88:A:LYS:HD2 | 12       | 0.13          |
| (1,238) | 1:55:B:GLU:H    | 1:20:B:VAL:HA  | 13       | 0.13          |
| (1,237) | 1:55:A:GLU:H    | 1:20:A:VAL:HA  | 13       | 0.13          |
| (1,228) | 1:63:B:PRO:HB3  | 1:64:B:VAL:H   | 14       | 0.13          |
| (1,227) | 1:63:A:PRO:HB3  | 1:64:A:VAL:H   | 14       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 1        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 2        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 3        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 4        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 5        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 6        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 7        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 8        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 9        | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 10       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 11       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 12       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 13       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 14       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 15       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 16       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 17       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 18       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 19       | 0.13          |
| (1,166) | 1:35:B:GLU:HG2  | 1:35:B:GLU:HG3 | 20       | 0.13          |
| (1,165) | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3 | 1        | 0.13          |
| (1,165) | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3 | 2        | 0.13          |
| (1,165) | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3 | 3        | 0.13          |
| (1,165) | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3 | 4        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 5        | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 6        | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 7        | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 8        | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 9        | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 10       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 11       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 12       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 13       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 14       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 15       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 16       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 17       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 18       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 19       | 0.13          |
| (1,165)  | 1:35:A:GLU:HG2  | 1:35:A:GLU:HG3   | 20       | 0.13          |
| (1,66)   | 1:32:B:LYS:HE2  | 1:32:B:LYS:HD2   | 19       | 0.13          |
| (1,65)   | 1:32:A:LYS:HE2  | 1:32:A:LYS:HD2   | 10       | 0.13          |
| (1,65)   | 1:32:A:LYS:HE2  | 1:32:A:LYS:HD2   | 19       | 0.13          |
| (1,6)    | 1:79:B:TYR:H    | 1:111:B:VAL:HG21 | 11       | 0.13          |
| (1,3101) | 1:9:A:ARG:HB3   | 1:115:B:LYS:HA   | 4        | 0.12          |
| (1,3092) | 1:86:B:PHE:H    | 1:54:A:PHE:HD1   | 5        | 0.12          |
| (1,3063) | 1:12:A:PHE:H    | 1:111:B:VAL:HG11 | 12       | 0.12          |
| (1,3055) | 1:107:A:ALA:HB1 | 1:109:B:VAL:HG11 | 14       | 0.12          |
| (1,3040) | 1:35:B:GLU:H    | 1:34:B:LYS:HD3   | 16       | 0.12          |
| (1,3039) | 1:35:A:GLU:H    | 1:34:A:LYS:HD3   | 16       | 0.12          |
| (1,3020) | 1:28:B:ALA:H    | 1:28:B:ALA:HB2   | 4        | 0.12          |
| (1,3019) | 1:28:A:ALA:H    | 1:28:A:ALA:HB2   | 4        | 0.12          |
| (1,3019) | 1:28:A:ALA:H    | 1:28:A:ALA:HB3   | 14       | 0.12          |
| (1,3004) | 1:28:B:ALA:H    | 1:38:B:VAL:HG11  | 17       | 0.12          |
| (1,3003) | 1:28:A:ALA:H    | 1:38:A:VAL:HG11  | 17       | 0.12          |
| (1,2906) | 1:22:B:VAL:H    | 1:53:B:PHE:HB3   | 19       | 0.12          |
| (1,2905) | 1:22:A:VAL:H    | 1:53:A:PHE:HB3   | 19       | 0.12          |
| (1,2854) | 1:73:B:SER:H    | 1:76:B:TRP:HB3   | 18       | 0.12          |
| (1,2853) | 1:73:A:SER:H    | 1:76:A:TRP:HB3   | 18       | 0.12          |
| (1,2764) | 1:18:B:VAL:H    | 1:108:B:CYS:HB3  | 10       | 0.12          |
| (1,2579) | 1:107:A:ALA:H   | 1:82:A:THR:HG21  | 12       | 0.12          |
| (1,2504) | 1:30:B:ASP:H    | 1:34:B:LYS:HB2   | 1        | 0.12          |
| (1,2503) | 1:30:A:ASP:H    | 1:34:A:LYS:HB2   | 1        | 0.12          |
| (1,2503) | 1:30:A:ASP:H    | 1:34:A:LYS:HB2   | 13       | 0.12          |
| (1,2387) | 1:29:A:THR:H    | 1:28:A:ALA:HB3   | 13       | 0.12          |
| (1,2224) | 1:118:B:ARG:H   | 1:118:B:ARG:HB2  | 11       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2126) | 1:32:B:LYS:H     | 1:31:B:ILE:HG12  | 7        | 0.12          |
| (1,2125) | 1:32:A:LYS:H     | 1:31:A:ILE:HG12  | 7        | 0.12          |
| (1,2112) | 1:117:B:VAL:H    | 1:116:B:ALA:HB2  | 20       | 0.12          |
| (1,2111) | 1:117:A:VAL:H    | 1:116:A:ALA:HB1  | 14       | 0.12          |
| (1,2111) | 1:117:A:VAL:H    | 1:116:A:ALA:HB2  | 20       | 0.12          |
| (1,2031) | 1:27:A:THR:H     | 1:38:A:VAL:HG22  | 17       | 0.12          |
| (1,1970) | 1:33:B:GLY:H     | 1:31:B:ILE:HG12  | 4        | 0.12          |
| (1,1969) | 1:33:A:GLY:H     | 1:31:A:ILE:HG12  | 4        | 0.12          |
| (1,1897) | 1:48:A:VAL:H     | 1:48:A:VAL:HG11  | 15       | 0.12          |
| (1,1881) | 1:21:A:TRP:H     | 1:21:A:TRP:HZ2   | 16       | 0.12          |
| (1,1880) | 1:21:B:TRP:H     | 1:20:B:VAL:HG23  | 6        | 0.12          |
| (1,1879) | 1:21:A:TRP:H     | 1:20:A:VAL:HG23  | 6        | 0.12          |
| (1,1740) | 1:36:B:VAL:H     | 1:27:B:THR:HG22  | 20       | 0.12          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG21  | 13       | 0.12          |
| (1,1739) | 1:36:A:VAL:H     | 1:27:A:THR:HG22  | 20       | 0.12          |
| (1,1722) | 1:76:B:TRP:H     | 1:115:B:LYS:HG2  | 11       | 0.12          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG23 | 14       | 0.12          |
| (1,1702) | 1:31:B:ILE:H     | 1:102:B:ILE:HG23 | 16       | 0.12          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG23 | 14       | 0.12          |
| (1,1701) | 1:31:A:ILE:H     | 1:102:A:ILE:HG23 | 16       | 0.12          |
| (1,1650) | 1:47:B:SER:H     | 1:48:B:VAL:HG12  | 8        | 0.12          |
| (1,1649) | 1:47:A:SER:H     | 1:48:A:VAL:HG12  | 5        | 0.12          |
| (1,1609) | 1:24:A:ASP:H     | 1:22:A:VAL:HG21  | 12       | 0.12          |
| (1,1555) | 1:49:A:PHE:HA    | 1:48:A:VAL:HB    | 1        | 0.12          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 11       | 0.12          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 11       | 0.12          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 17       | 0.12          |
| (1,1472) | 1:112:B:LEU:HD21 | 1:112:B:LEU:HD11 | 18       | 0.12          |
| (1,1471) | 1:112:A:LEU:HD21 | 1:112:A:LEU:HD11 | 18       | 0.12          |
| (1,1450) | 1:25:B:LYS:HG2   | 1:53:B:PHE:HE1   | 16       | 0.12          |
| (1,1362) | 1:104:B:ILE:HB   | 1:87:B:VAL:HG22  | 9        | 0.12          |
| (1,1361) | 1:104:A:ILE:HB   | 1:87:A:VAL:HG22  | 9        | 0.12          |
| (1,1348) | 1:87:B:VAL:HG12  | 1:104:B:ILE:HD12 | 1        | 0.12          |
| (1,1348) | 1:87:B:VAL:HG12  | 1:104:B:ILE:HD11 | 3        | 0.12          |
| (1,1348) | 1:87:B:VAL:HG12  | 1:104:B:ILE:HD11 | 10       | 0.12          |
| (1,1347) | 1:87:A:VAL:HG12  | 1:104:A:ILE:HD12 | 1        | 0.12          |
| (1,1347) | 1:87:A:VAL:HG12  | 1:104:A:ILE:HD11 | 3        | 0.12          |
| (1,1266) | 1:70:B:GLY:HA2   | 1:71:B:ILE:HD11  | 1        | 0.12          |
| (1,1266) | 1:70:B:GLY:HA2   | 1:71:B:ILE:HD12  | 12       | 0.12          |
| (1,1265) | 1:70:A:GLY:HA2   | 1:71:A:ILE:HD11  | 1        | 0.12          |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 13       | 0.12          |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 13       | 0.12          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 1        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 2        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 3        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 4        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 5        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 6        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 7        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 8        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 9        | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 10       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 11       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 12       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 13       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 14       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 15       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 16       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 17       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 18       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 19       | 0.12          |
| (1,1024) | 1:13:B:SER:HB3 | 1:13:B:SER:HB2   | 20       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 1        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 2        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 3        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 4        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 5        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 6        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 7        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 8        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 9        | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 10       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 11       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 12       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 13       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 14       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 15       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 16       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 17       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 18       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 19       | 0.12          |
| (1,1023) | 1:13:A:SER:HB3 | 1:13:A:SER:HB2   | 20       | 0.12          |
| (1,927)  | 1:111:A:VAL:HB | 1:111:A:VAL:HG12 | 5        | 0.12          |
| (1,920)  | 1:117:B:VAL:HB | 1:116:B:ALA:HB1  | 4        | 0.12          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,919) | 1:117:A:VAL:HB   | 1:116:A:ALA:HB1 | 4        | 0.12          |
| (1,853) | 1:37:A:MET:HG3   | 1:36:A:VAL:HA   | 2        | 0.12          |
| (1,712) | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2  | 10       | 0.12          |
| (1,712) | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2  | 15       | 0.12          |
| (1,711) | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2  | 15       | 0.12          |
| (1,604) | 1:104:B:ILE:HB   | 1:85:B:THR:HG21 | 19       | 0.12          |
| (1,603) | 1:104:A:ILE:HB   | 1:85:A:THR:HG21 | 19       | 0.12          |
| (1,594) | 1:108:B:CYS:H    | 1:107:B:ALA:HB2 | 3        | 0.12          |
| (1,460) | 1:43:B:ASN:HB3   | 1:44:B:ILE:HG12 | 11       | 0.12          |
| (1,459) | 1:43:A:ASN:HB3   | 1:44:A:ILE:HG12 | 11       | 0.12          |
| (1,334) | 1:36:B:VAL:HG12  | 1:36:B:VAL:HB   | 1        | 0.12          |
| (1,334) | 1:36:B:VAL:HG11  | 1:36:B:VAL:HB   | 2        | 0.12          |
| (1,334) | 1:36:B:VAL:HG12  | 1:36:B:VAL:HB   | 3        | 0.12          |
| (1,334) | 1:36:B:VAL:HG11  | 1:36:B:VAL:HB   | 6        | 0.12          |
| (1,334) | 1:36:B:VAL:HG13  | 1:36:B:VAL:HB   | 8        | 0.12          |
| (1,334) | 1:36:B:VAL:HG12  | 1:36:B:VAL:HB   | 9        | 0.12          |
| (1,334) | 1:36:B:VAL:HG12  | 1:36:B:VAL:HB   | 10       | 0.12          |
| (1,334) | 1:36:B:VAL:HG13  | 1:36:B:VAL:HB   | 12       | 0.12          |
| (1,334) | 1:36:B:VAL:HG13  | 1:36:B:VAL:HB   | 13       | 0.12          |
| (1,334) | 1:36:B:VAL:HG11  | 1:36:B:VAL:HB   | 14       | 0.12          |
| (1,334) | 1:36:B:VAL:HG12  | 1:36:B:VAL:HB   | 15       | 0.12          |
| (1,334) | 1:36:B:VAL:HG12  | 1:36:B:VAL:HB   | 19       | 0.12          |
| (1,333) | 1:36:A:VAL:HG12  | 1:36:A:VAL:HB   | 1        | 0.12          |
| (1,333) | 1:36:A:VAL:HG11  | 1:36:A:VAL:HB   | 2        | 0.12          |
| (1,333) | 1:36:A:VAL:HG12  | 1:36:A:VAL:HB   | 3        | 0.12          |
| (1,333) | 1:36:A:VAL:HG11  | 1:36:A:VAL:HB   | 6        | 0.12          |
| (1,333) | 1:36:A:VAL:HG13  | 1:36:A:VAL:HB   | 8        | 0.12          |
| (1,333) | 1:36:A:VAL:HG12  | 1:36:A:VAL:HB   | 9        | 0.12          |
| (1,333) | 1:36:A:VAL:HG12  | 1:36:A:VAL:HB   | 10       | 0.12          |
| (1,333) | 1:36:A:VAL:HG13  | 1:36:A:VAL:HB   | 12       | 0.12          |
| (1,333) | 1:36:A:VAL:HG13  | 1:36:A:VAL:HB   | 13       | 0.12          |
| (1,333) | 1:36:A:VAL:HG11  | 1:36:A:VAL:HB   | 14       | 0.12          |
| (1,333) | 1:36:A:VAL:HG12  | 1:36:A:VAL:HB   | 15       | 0.12          |
| (1,333) | 1:36:A:VAL:HG12  | 1:36:A:VAL:HB   | 19       | 0.12          |
| (1,282) | 1:37:B:MET:HA    | 1:37:B:MET:HE3  | 17       | 0.12          |
| (1,281) | 1:37:A:MET:HA    | 1:37:A:MET:HE3  | 17       | 0.12          |
| (1,257) | 1:112:A:LEU:HD21 | 1:76:A:TRP:HB2  | 4        | 0.12          |
| (1,234) | 1:33:B:GLY:HA2   | 1:29:B:THR:HB   | 7        | 0.12          |
| (1,233) | 1:33:A:GLY:HA2   | 1:29:A:THR:HB   | 7        | 0.12          |
| (1,228) | 1:63:B:PRO:HB3   | 1:64:B:VAL:H    | 2        | 0.12          |
| (1,228) | 1:63:B:PRO:HB3   | 1:64:B:VAL:H    | 9        | 0.12          |
| (1,227) | 1:63:A:PRO:HB3   | 1:64:A:VAL:H    | 2        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,227)  | 1:63:A:PRO:HB3  | 1:64:A:VAL:H     | 9        | 0.12          |
| (1,66)   | 1:32:B:LYS:HE2  | 1:32:B:LYS:HD2   | 10       | 0.12          |
| (1,6)    | 1:79:B:TYR:H    | 1:111:B:VAL:HG23 | 12       | 0.12          |
| (1,5)    | 1:79:A:TYR:H    | 1:111:A:VAL:HG23 | 12       | 0.12          |
| (1,3020) | 1:28:B:ALA:H    | 1:28:B:ALA:HB3   | 14       | 0.11          |
| (1,3014) | 1:28:B:ALA:H    | 1:29:B:THR:HA    | 9        | 0.11          |
| (1,3013) | 1:28:A:ALA:H    | 1:29:A:THR:HA    | 9        | 0.11          |
| (1,2988) | 1:103:B:ARG:H   | 1:102:B:ILE:HG13 | 10       | 0.11          |
| (1,2987) | 1:103:A:ARG:H   | 1:102:A:ILE:HG13 | 10       | 0.11          |
| (1,2976) | 1:103:B:ARG:H   | 1:103:B:ARG:HG2  | 3        | 0.11          |
| (1,2720) | 1:84:B:HIS:H    | 1:83:B:THR:HB    | 8        | 0.11          |
| (1,2719) | 1:84:A:HIS:H    | 1:83:A:THR:HB    | 8        | 0.11          |
| (1,2588) | 1:107:B:ALA:H   | 1:107:B:ALA:HB3  | 13       | 0.11          |
| (1,2580) | 1:107:B:ALA:H   | 1:82:B:THR:HG21  | 12       | 0.11          |
| (1,2432) | 1:92:B:MET:H    | 1:37:B:MET:HB2   | 13       | 0.11          |
| (1,2431) | 1:92:A:MET:H    | 1:37:A:MET:HB2   | 13       | 0.11          |
| (1,2223) | 1:118:A:ARG:H   | 1:118:A:ARG:HB2  | 11       | 0.11          |
| (1,1914) | 1:72:B:ASP:H    | 1:71:B:ILE:HA    | 4        | 0.11          |
| (1,1913) | 1:72:A:ASP:H    | 1:71:A:ILE:HA    | 4        | 0.11          |
| (1,1912) | 1:72:B:ASP:H    | 1:76:B:TRP:HB3   | 18       | 0.11          |
| (1,1911) | 1:72:A:ASP:H    | 1:76:A:TRP:HB3   | 18       | 0.11          |
| (1,1898) | 1:48:B:VAL:H    | 1:48:B:VAL:HG13  | 14       | 0.11          |
| (1,1880) | 1:21:B:TRP:H    | 1:20:B:VAL:HG21  | 5        | 0.11          |
| (1,1880) | 1:21:B:TRP:H    | 1:20:B:VAL:HG21  | 20       | 0.11          |
| (1,1879) | 1:21:A:TRP:H    | 1:20:A:VAL:HG21  | 5        | 0.11          |
| (1,1879) | 1:21:A:TRP:H    | 1:20:A:VAL:HG21  | 20       | 0.11          |
| (1,1740) | 1:36:B:VAL:H    | 1:27:B:THR:HG21  | 10       | 0.11          |
| (1,1739) | 1:36:A:VAL:H    | 1:27:A:THR:HG21  | 10       | 0.11          |
| (1,1649) | 1:47:A:SER:H    | 1:48:A:VAL:HG12  | 8        | 0.11          |
| (1,1556) | 1:49:B:PHE:HA   | 1:48:B:VAL:HB    | 1        | 0.11          |
| (1,1554) | 1:48:B:VAL:HG22 | 1:48:B:VAL:HB    | 2        | 0.11          |
| (1,1554) | 1:48:B:VAL:HG22 | 1:48:B:VAL:HB    | 3        | 0.11          |
| (1,1554) | 1:48:B:VAL:HG23 | 1:48:B:VAL:HB    | 7        | 0.11          |
| (1,1554) | 1:48:B:VAL:HG22 | 1:48:B:VAL:HB    | 8        | 0.11          |
| (1,1554) | 1:48:B:VAL:HG23 | 1:48:B:VAL:HB    | 10       | 0.11          |
| (1,1554) | 1:48:B:VAL:HG23 | 1:48:B:VAL:HB    | 17       | 0.11          |
| (1,1554) | 1:48:B:VAL:HG22 | 1:48:B:VAL:HB    | 19       | 0.11          |
| (1,1553) | 1:48:A:VAL:HG22 | 1:48:A:VAL:HB    | 2        | 0.11          |
| (1,1553) | 1:48:A:VAL:HG22 | 1:48:A:VAL:HB    | 3        | 0.11          |
| (1,1553) | 1:48:A:VAL:HG23 | 1:48:A:VAL:HB    | 4        | 0.11          |
| (1,1553) | 1:48:A:VAL:HG22 | 1:48:A:VAL:HB    | 8        | 0.11          |
| (1,1553) | 1:48:A:VAL:HG22 | 1:48:A:VAL:HB    | 10       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1553) | 1:48:A:VAL:HG21  | 1:48:A:VAL:HB    | 16       | 0.11          |
| (1,1553) | 1:48:A:VAL:HG23  | 1:48:A:VAL:HB    | 17       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 1        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 2        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 3        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 4        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 5        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 6        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 7        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 8        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 9        | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 10       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 12       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 13       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 14       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 15       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 16       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 17       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 18       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 19       | 0.11          |
| (1,1532) | 1:67:B:GLY:HA3   | 1:67:B:GLY:HA2   | 20       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 1        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 2        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 3        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 4        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 5        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 6        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 7        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 8        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 9        | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 10       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 12       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 13       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 14       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 15       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 16       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 18       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 19       | 0.11          |
| (1,1531) | 1:67:A:GLY:HA3   | 1:67:A:GLY:HA2   | 20       | 0.11          |
| (1,1490) | 1:110:B:CYS:HB3  | 1:14:B:VAL:HG22  | 1        | 0.11          |
| (1,1489) | 1:110:A:CYS:HB3  | 1:14:A:VAL:HG22  | 1        | 0.11          |
| (1,1472) | 1:112:B:LEU:HD21 | 1:112:B:LEU:HD13 | 16       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1472) | 1:112:B:LEU:HD21 | 1:112:B:LEU:HD13 | 20       | 0.11          |
| (1,1471) | 1:112:A:LEU:HD21 | 1:112:A:LEU:HD13 | 16       | 0.11          |
| (1,1449) | 1:25:A:LYS:HG2   | 1:53:A:PHE:HE1   | 16       | 0.11          |
| (1,1420) | 1:6:B:ILE:HG12   | 1:6:B:ILE:HG23   | 14       | 0.11          |
| (1,1420) | 1:6:B:ILE:HG12   | 1:6:B:ILE:HG23   | 15       | 0.11          |
| (1,1419) | 1:6:A:ILE:HG12   | 1:6:A:ILE:HG23   | 14       | 0.11          |
| (1,1419) | 1:6:A:ILE:HG12   | 1:6:A:ILE:HG23   | 15       | 0.11          |
| (1,1400) | 1:59:B:ARG:HG2   | 1:18:B:VAL:HG11  | 18       | 0.11          |
| (1,1399) | 1:59:A:ARG:HG2   | 1:18:A:VAL:HG11  | 18       | 0.11          |
| (1,1362) | 1:104:B:ILE:HB   | 1:87:B:VAL:HG22  | 6        | 0.11          |
| (1,1362) | 1:104:B:ILE:HB   | 1:87:B:VAL:HG21  | 13       | 0.11          |
| (1,1361) | 1:104:A:ILE:HB   | 1:87:A:VAL:HG22  | 6        | 0.11          |
| (1,1265) | 1:70:A:GLY:HA2   | 1:71:A:ILE:HD12  | 12       | 0.11          |
| (1,1170) | 1:39:B:LEU:HD13  | 1:92:B:MET:HG2   | 13       | 0.11          |
| (1,1170) | 1:39:B:LEU:HD13  | 1:92:B:MET:HG2   | 16       | 0.11          |
| (1,1169) | 1:39:A:LEU:HD13  | 1:92:A:MET:HG2   | 13       | 0.11          |
| (1,1064) | 1:57:B:LYS:HD2   | 1:57:B:LYS:HB2   | 2        | 0.11          |
| (1,1063) | 1:57:A:LYS:HD2   | 1:57:A:LYS:HB2   | 2        | 0.11          |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG12 | 2        | 0.11          |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG13 | 3        | 0.11          |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG12 | 5        | 0.11          |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG11 | 6        | 0.11          |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG13 | 3        | 0.11          |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG11 | 6        | 0.11          |
| (1,854)  | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 2        | 0.11          |
| (1,854)  | 1:37:B:MET:HG3   | 1:36:B:VAL:HA    | 4        | 0.11          |
| (1,853)  | 1:37:A:MET:HG3   | 1:36:A:VAL:HA    | 4        | 0.11          |
| (1,810)  | 1:118:B:ARG:HB2  | 1:118:B:ARG:HG2  | 20       | 0.11          |
| (1,809)  | 1:118:A:ARG:HB2  | 1:118:A:ARG:HG2  | 20       | 0.11          |
| (1,712)  | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 6        | 0.11          |
| (1,711)  | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 3        | 0.11          |
| (1,662)  | 1:42:B:VAL:HG13  | 1:90:B:LEU:HG    | 12       | 0.11          |
| (1,661)  | 1:42:A:VAL:HG13  | 1:90:A:LEU:HG    | 12       | 0.11          |
| (1,600)  | 1:107:B:ALA:HB2  | 1:107:B:ALA:HA   | 19       | 0.11          |
| (1,418)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HB    | 6        | 0.11          |
| (1,418)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HB    | 11       | 0.11          |
| (1,418)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HB    | 12       | 0.11          |
| (1,418)  | 1:38:B:VAL:HG12  | 1:38:B:VAL:HB    | 14       | 0.11          |
| (1,418)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HB    | 18       | 0.11          |
| (1,417)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HB    | 6        | 0.11          |
| (1,417)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HB    | 11       | 0.11          |
| (1,417)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HB    | 12       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,417)  | 1:38:A:VAL:HG12  | 1:38:A:VAL:HB    | 14       | 0.11          |
| (1,417)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HB    | 18       | 0.11          |
| (1,344)  | 1:48:B:VAL:HG11  | 1:41:B:GLU:HG2   | 6        | 0.11          |
| (1,340)  | 1:28:B:ALA:H     | 1:36:B:VAL:HG12  | 5        | 0.11          |
| (1,339)  | 1:28:A:ALA:H     | 1:36:A:VAL:HG12  | 5        | 0.11          |
| (1,272)  | 1:14:B:VAL:HG12  | 1:15:B:CYS:HB2   | 16       | 0.11          |
| (1,271)  | 1:14:A:VAL:HG12  | 1:15:A:CYS:HB2   | 16       | 0.11          |
| (1,270)  | 1:14:B:VAL:HG11  | 1:110:B:CYS:HB3  | 15       | 0.11          |
| (1,269)  | 1:14:A:VAL:HG11  | 1:110:A:CYS:HB3  | 15       | 0.11          |
| (1,258)  | 1:112:B:LEU:HD21 | 1:76:B:TRP:HB2   | 4        | 0.11          |
| (1,250)  | 1:112:B:LEU:HD22 | 1:76:B:TRP:HD1   | 9        | 0.11          |
| (1,249)  | 1:112:A:LEU:HD22 | 1:76:A:TRP:HD1   | 9        | 0.11          |
| (1,3094) | 1:86:B:PHE:H     | 1:54:A:PHE:HE2   | 7        | 0.1           |
| (1,3064) | 1:12:B:PHE:H     | 1:111:A:VAL:HG11 | 12       | 0.1           |
| (1,2988) | 1:103:B:ARG:H    | 1:102:B:ILE:HG13 | 3        | 0.1           |
| (1,2987) | 1:103:A:ARG:H    | 1:102:A:ILE:HG13 | 3        | 0.1           |
| (1,2975) | 1:103:A:ARG:H    | 1:103:A:ARG:HG2  | 3        | 0.1           |
| (1,2764) | 1:18:B:VAL:H     | 1:108:B:CYS:HB3  | 20       | 0.1           |
| (1,2763) | 1:18:A:VAL:H     | 1:108:A:CYS:HB3  | 20       | 0.1           |
| (1,2587) | 1:107:A:ALA:H    | 1:107:A:ALA:HB3  | 13       | 0.1           |
| (1,2384) | 1:29:B:THR:H     | 1:30:B:ASP:HB2   | 8        | 0.1           |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG11 | 4        | 0.1           |
| (1,2232) | 1:118:B:ARG:H    | 1:117:B:VAL:HG12 | 14       | 0.1           |
| (1,2231) | 1:118:A:ARG:H    | 1:117:A:VAL:HG11 | 4        | 0.1           |
| (1,2112) | 1:117:B:VAL:H    | 1:116:B:ALA:HB2  | 16       | 0.1           |
| (1,2111) | 1:117:A:VAL:H    | 1:116:A:ALA:HB2  | 16       | 0.1           |
| (1,2056) | 1:53:B:PHE:H     | 1:53:B:PHE:HB3   | 20       | 0.1           |
| (1,2055) | 1:53:A:PHE:H     | 1:53:A:PHE:HB3   | 20       | 0.1           |
| (1,1996) | 1:67:B:GLY:H     | 1:64:B:VAL:HB    | 8        | 0.1           |
| (1,1898) | 1:48:B:VAL:H     | 1:48:B:VAL:HG12  | 1        | 0.1           |
| (1,1897) | 1:48:A:VAL:H     | 1:48:A:VAL:HG13  | 14       | 0.1           |
| (1,1554) | 1:48:B:VAL:HG22  | 1:48:B:VAL:HB    | 1        | 0.1           |
| (1,1554) | 1:48:B:VAL:HG23  | 1:48:B:VAL:HB    | 4        | 0.1           |
| (1,1554) | 1:48:B:VAL:HG23  | 1:48:B:VAL:HB    | 11       | 0.1           |
| (1,1554) | 1:48:B:VAL:HG22  | 1:48:B:VAL:HB    | 12       | 0.1           |
| (1,1554) | 1:48:B:VAL:HG22  | 1:48:B:VAL:HB    | 13       | 0.1           |
| (1,1554) | 1:48:B:VAL:HG21  | 1:48:B:VAL:HB    | 16       | 0.1           |
| (1,1553) | 1:48:A:VAL:HG21  | 1:48:A:VAL:HB    | 5        | 0.1           |
| (1,1553) | 1:48:A:VAL:HG23  | 1:48:A:VAL:HB    | 7        | 0.1           |
| (1,1553) | 1:48:A:VAL:HG23  | 1:48:A:VAL:HB    | 11       | 0.1           |
| (1,1553) | 1:48:A:VAL:HG22  | 1:48:A:VAL:HB    | 12       | 0.1           |
| (1,1553) | 1:48:A:VAL:HG22  | 1:48:A:VAL:HB    | 13       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1553) | 1:48:A:VAL:HG23  | 1:48:A:VAL:HB    | 19       | 0.1           |
| (1,1553) | 1:48:A:VAL:HG22  | 1:48:A:VAL:HB    | 20       | 0.1           |
| (1,1471) | 1:112:A:LEU:HD21 | 1:112:A:LEU:HD13 | 20       | 0.1           |
| (1,1361) | 1:104:A:ILE:HB   | 1:87:A:VAL:HG21  | 13       | 0.1           |
| (1,1314) | 1:70:B:GLY:H     | 1:64:B:VAL:HG12  | 15       | 0.1           |
| (1,1313) | 1:70:A:GLY:H     | 1:64:A:VAL:HG12  | 15       | 0.1           |
| (1,1252) | 1:68:B:CYS:HB3   | 1:14:B:VAL:HB    | 12       | 0.1           |
| (1,1251) | 1:68:A:CYS:HB3   | 1:14:A:VAL:HB    | 12       | 0.1           |
| (1,1170) | 1:39:B:LEU:HD11  | 1:92:B:MET:HG2   | 14       | 0.1           |
| (1,1169) | 1:39:A:LEU:HD13  | 1:92:A:MET:HG2   | 10       | 0.1           |
| (1,1169) | 1:39:A:LEU:HD13  | 1:92:A:MET:HG2   | 16       | 0.1           |
| (1,988)  | 1:27:B:THR:HG21  | 1:35:B:GLU:HG3   | 3        | 0.1           |
| (1,987)  | 1:27:A:THR:HG21  | 1:35:A:GLU:HG3   | 3        | 0.1           |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG12 | 11       | 0.1           |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG13 | 13       | 0.1           |
| (1,928)  | 1:111:B:VAL:HB   | 1:111:B:VAL:HG13 | 14       | 0.1           |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG12 | 2        | 0.1           |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG12 | 9        | 0.1           |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG13 | 13       | 0.1           |
| (1,927)  | 1:111:A:VAL:HB   | 1:111:A:VAL:HG13 | 14       | 0.1           |
| (1,874)  | 1:39:B:LEU:HD12  | 1:91:B:THR:HA    | 12       | 0.1           |
| (1,712)  | 1:34:B:LYS:HB2   | 1:34:B:LYS:HD2   | 3        | 0.1           |
| (1,711)  | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 5        | 0.1           |
| (1,711)  | 1:34:A:LYS:HB2   | 1:34:A:LYS:HD2   | 6        | 0.1           |
| (1,600)  | 1:107:B:ALA:HB1  | 1:107:B:ALA:HA   | 4        | 0.1           |
| (1,600)  | 1:107:B:ALA:HB1  | 1:107:B:ALA:HA   | 8        | 0.1           |
| (1,600)  | 1:107:B:ALA:HB2  | 1:107:B:ALA:HA   | 13       | 0.1           |
| (1,599)  | 1:107:A:ALA:HB2  | 1:107:A:ALA:HA   | 1        | 0.1           |
| (1,599)  | 1:107:A:ALA:HB1  | 1:107:A:ALA:HA   | 4        | 0.1           |
| (1,599)  | 1:107:A:ALA:HB1  | 1:107:A:ALA:HA   | 8        | 0.1           |
| (1,599)  | 1:107:A:ALA:HB2  | 1:107:A:ALA:HA   | 19       | 0.1           |
| (1,418)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HB    | 2        | 0.1           |
| (1,418)  | 1:38:B:VAL:HG11  | 1:38:B:VAL:HB    | 9        | 0.1           |
| (1,418)  | 1:38:B:VAL:HG13  | 1:38:B:VAL:HB    | 19       | 0.1           |
| (1,417)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HB    | 2        | 0.1           |
| (1,417)  | 1:38:A:VAL:HG11  | 1:38:A:VAL:HB    | 9        | 0.1           |
| (1,417)  | 1:38:A:VAL:HG13  | 1:38:A:VAL:HB    | 19       | 0.1           |
| (1,379)  | 1:104:A:ILE:HG21 | 1:104:A:ILE:HG12 | 9        | 0.1           |
| (1,334)  | 1:36:B:VAL:HG11  | 1:36:B:VAL:HB    | 5        | 0.1           |
| (1,333)  | 1:36:A:VAL:HG11  | 1:36:A:VAL:HB    | 5        | 0.1           |
| (1,281)  | 1:37:A:MET:HA    | 1:37:A:MET:HE3   | 6        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found