



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:04 AM UTC

PDB ID : 2N3J / pdb\_00002n3j  
BMRB ID : 25645  
Title : Solution Structure of the alpha-crystallin domain from the redox-sensitive chaperone, HSPB1  
Authors : Rajagopal, P.; Liu, Y.; Shi, L.; Klevit, R.E.  
Deposited on : 2015-06-03

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

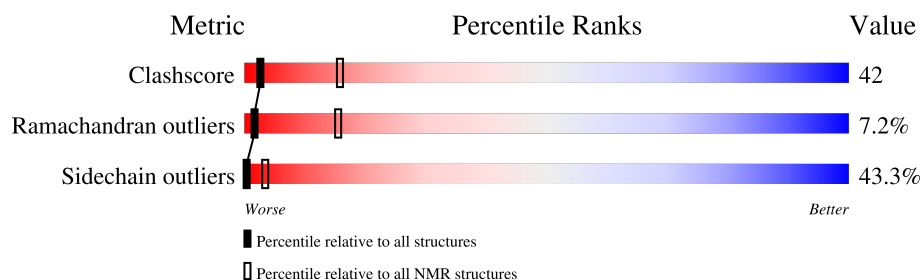
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 20%.

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     | 98     |                  |
| 1   | B     | 98     |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |                                              |                   |              |
|--------------------------------------|----------------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                        | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:94-A:127, A:132-A:170,<br>B:94-B:169 (149) | 0.77              | 7            |

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

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

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

| Cluster number        | Models      |
|-----------------------|-------------|
| 1                     | 3, 7, 8, 10 |
| 2                     | 2, 4, 5     |
| Single-model clusters | 1; 6; 9     |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3026 atoms, of which 1498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein beta-1.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 98       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1513  | 472 | 749 | 135 | 154 | 3 |       |
| 1   | B     | 98       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1513  | 472 | 749 | 135 | 154 | 3 |       |

There are 2 discrepancies between the modelled and reference sequences:

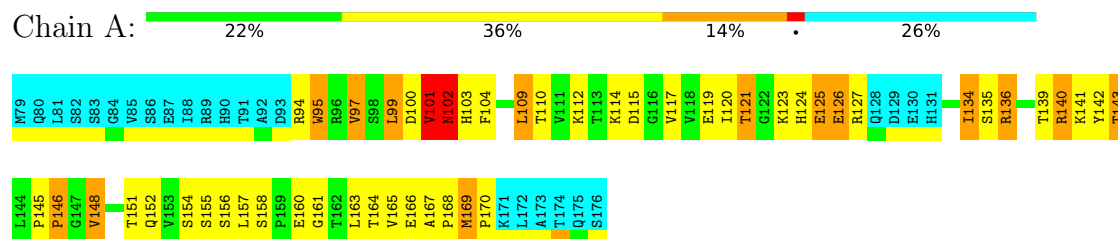
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 79      | MET      | -      | initiating methionine | UNP P04792 |
| B     | 79      | MET      | -      | initiating methionine | UNP P04792 |

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

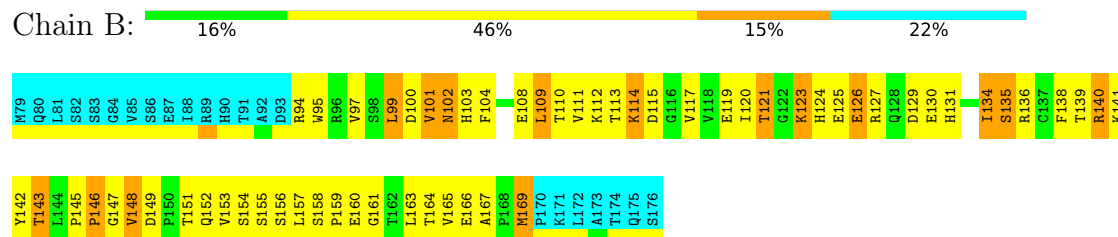
### 4.1 Average score per residue in the NMR ensemble

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: Heat shock protein beta-1



- Molecule 1: Heat shock protein beta-1

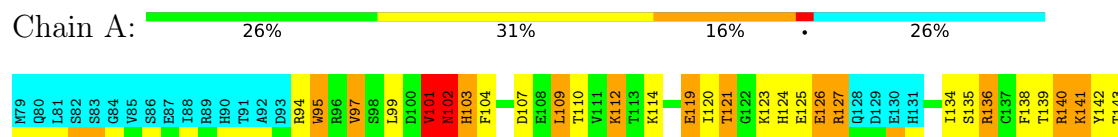


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

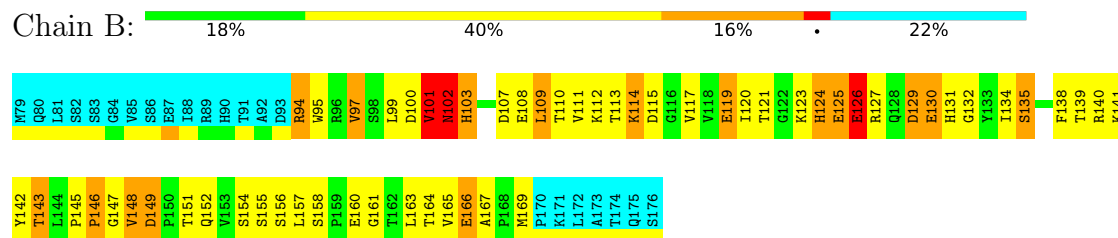
#### 4.2.1 Score per residue for model 1

- Molecule 1: Heat shock protein beta-1



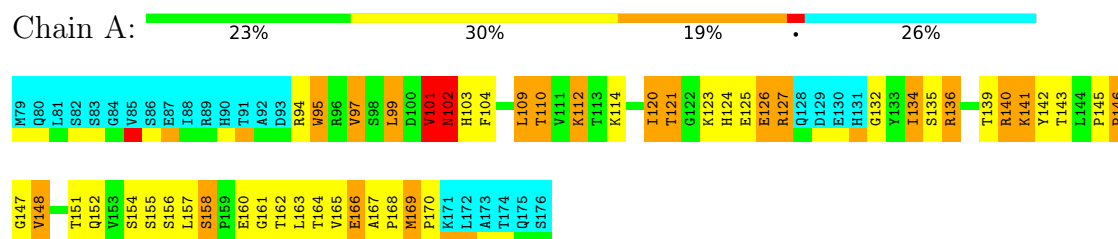


- Molecule 1: Heat shock protein beta-1

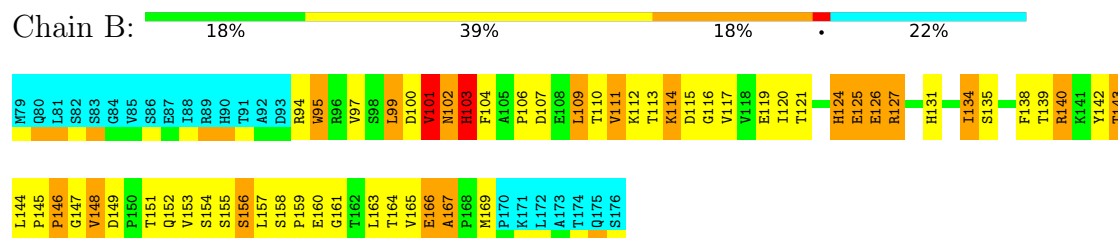


#### 4.2.2 Score per residue for model 2

- Molecule 1: Heat shock protein beta-1

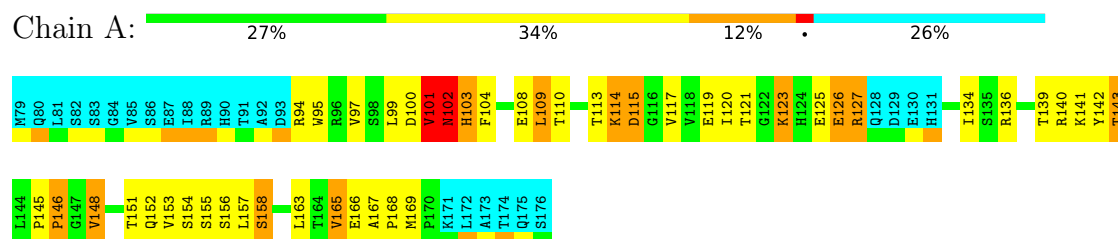


- Molecule 1: Heat shock protein beta-1

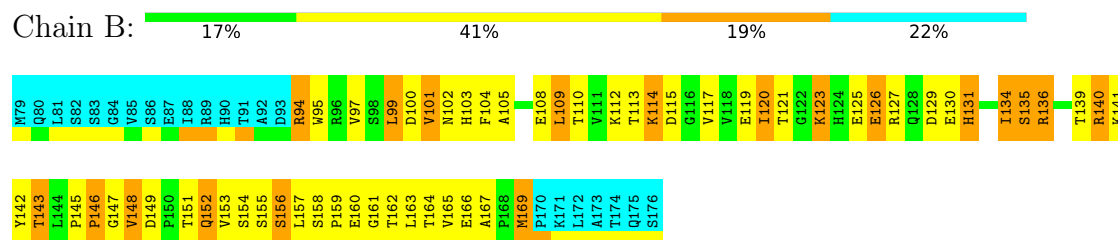


#### 4.2.3 Score per residue for model 3

- Molecule 1: Heat shock protein beta-1

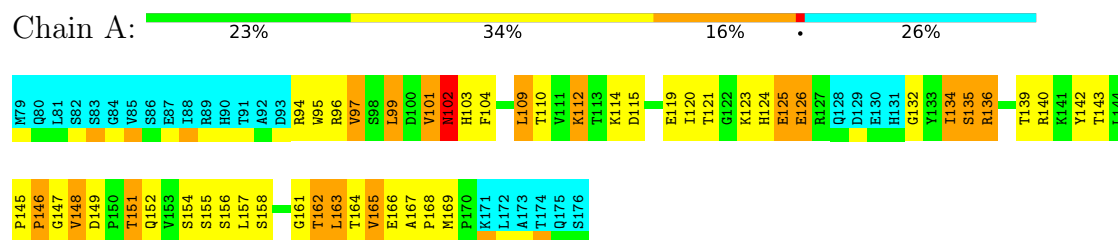


- Molecule 1: Heat shock protein beta-1

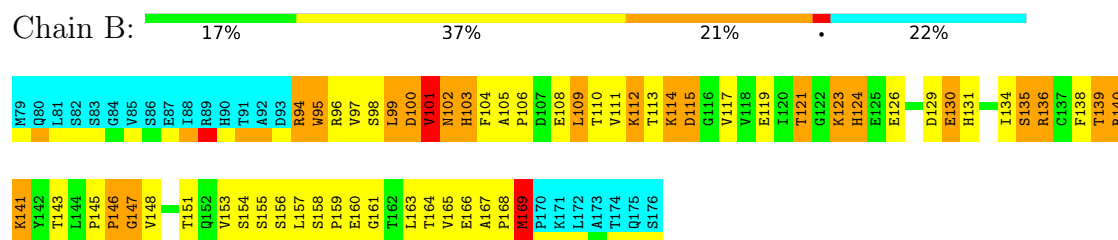


#### 4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein beta-1

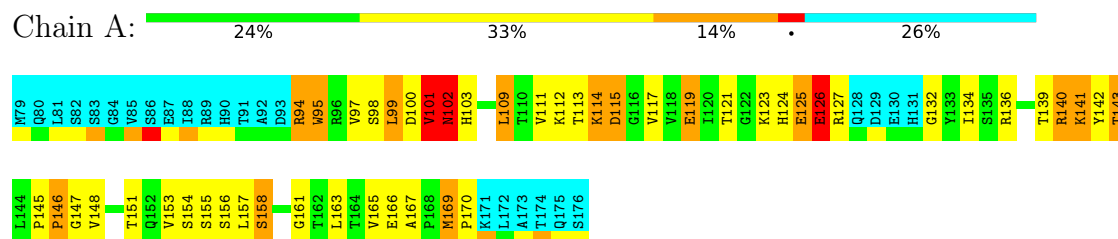


- Molecule 1: Heat shock protein beta-1

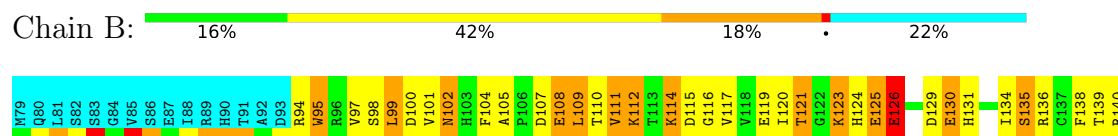


#### 4.2.5 Score per residue for model 5

- Molecule 1: Heat shock protein beta-1



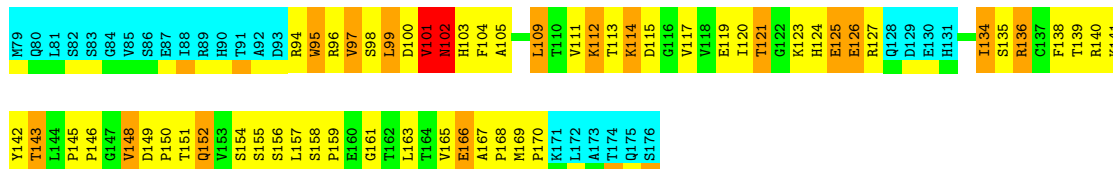
- Molecule 1: Heat shock protein beta-1



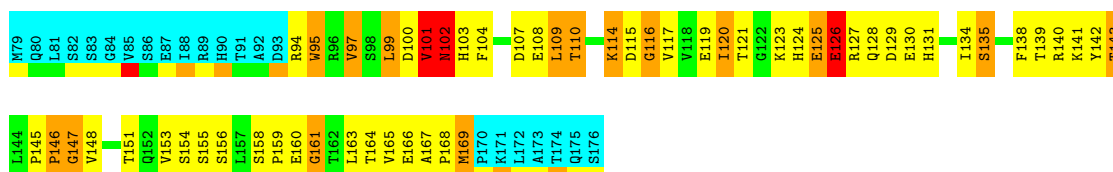
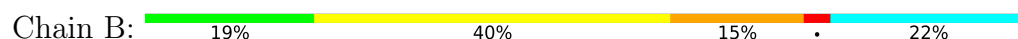


#### 4.2.6 Score per residue for model 6

- Molecule 1: Heat shock protein beta-1

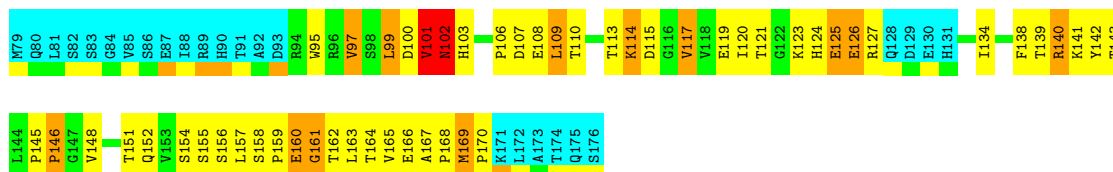
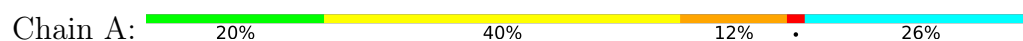


- Molecule 1: Heat shock protein beta-1

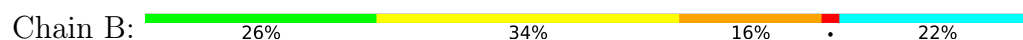


#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Heat shock protein beta-1



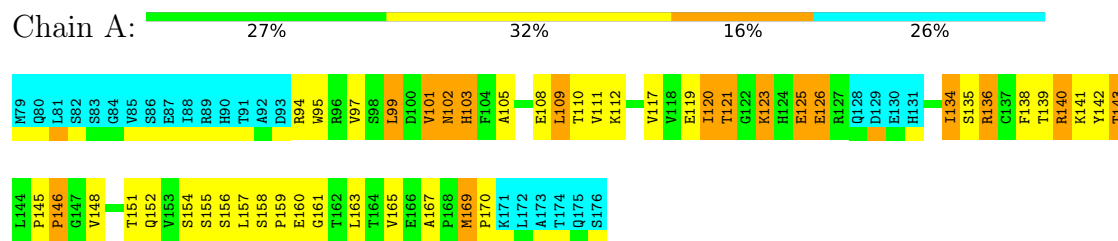
- Molecule 1: Heat shock protein beta-1



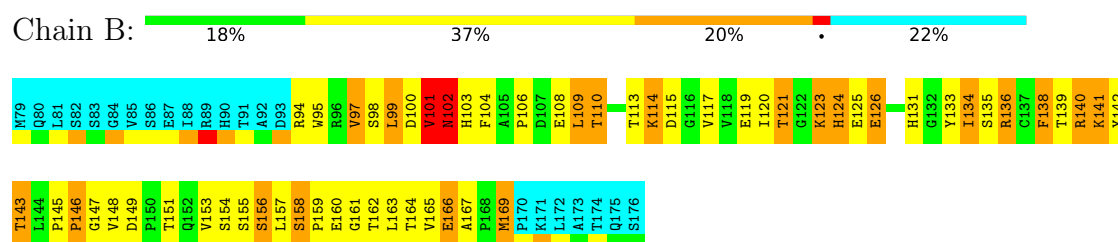


### 4.2.8 Score per residue for model 8

- Molecule 1: Heat shock protein beta-1

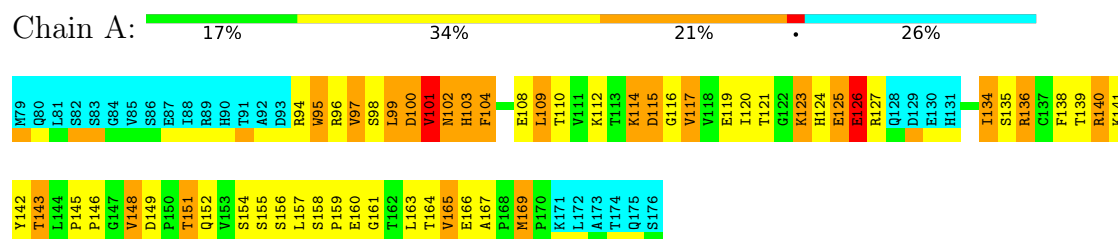


- Molecule 1: Heat shock protein beta-1

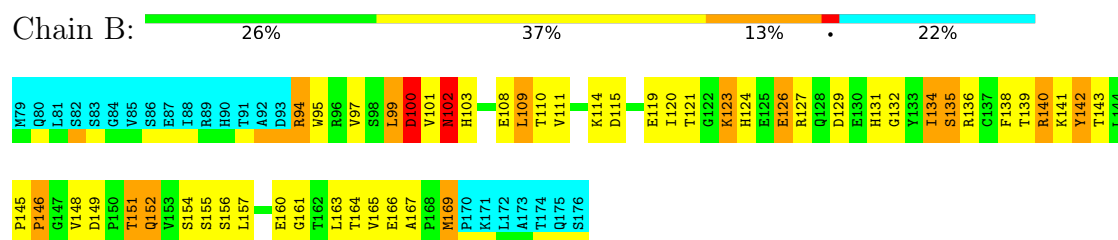


### 4.2.9 Score per residue for model 9

- Molecule 1: Heat shock protein beta-1

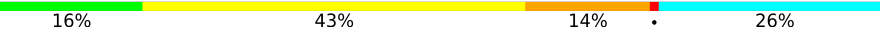


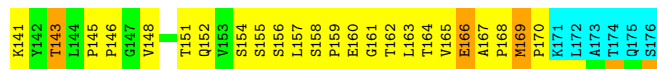
- Molecule 1: Heat shock protein beta-1



### 4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein beta-1

Chain A: 



● Molecule 1: Heat shock protein beta-1

Chain B: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CS-ROSETTA    | structure solution |         |
| X-PLOR NIH    | structure solution |         |
| X-PLOR NIH    | refinement         |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 490            |
| Number of shifts mapped to atoms             | 490            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 20%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.89±0.01    | 0±0/586 ( 0.0± 0.0%) | 1.02±0.02   | 0±0/800 ( 0.0± 0.0%) |
| 1   | B     | 0.88±0.02    | 0±0/615 ( 0.0± 0.0%) | 1.05±0.02   | 1±1/839 ( 0.1± 0.1%) |
| All | All   | 0.89         | 0/12010 ( 0.0%)      | 1.04        | 8/16390 ( 0.0%)      |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 1   | B     | 131 | HIS  | CA-CB-CG | -6.21 | 107.59      | 113.80   | 9      | 2     |
| 1   | B     | 167 | ALA  | N-CA-C   | 5.66  | 113.22      | 108.13   | 2      | 1     |
| 1   | B     | 124 | HIS  | CA-CB-CG | -5.58 | 108.22      | 113.80   | 2      | 2     |
| 1   | A     | 124 | HIS  | CA-CB-CG | -5.40 | 108.40      | 113.80   | 5      | 1     |
| 1   | B     | 103 | HIS  | CA-CB-CG | -5.39 | 108.41      | 113.80   | 2      | 1     |
| 1   | B     | 116 | GLY  | N-CA-C   | -5.03 | 108.76      | 115.40   | 6      | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 571   | 565      | 565      | 48±8    |
| 1   | B     | 600   | 583      | 583      | 53±7    |
| All | All   | 11710 | 11480    | 11480    | 972     |

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 42.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:117:VAL:HG22 | 1:B:143:THR:HG23 | 0.85     | 1.47        | 4      | 6     |
| 1:A:102:ASN:HB3  | 1:A:109:LEU:HD13 | 0.79     | 1.53        | 1      | 4     |
| 1:B:99:LEU:HD22  | 1:B:120:ILE:HG12 | 0.79     | 1.52        | 6      | 3     |
| 1:B:102:ASN:HB3  | 1:B:109:LEU:HD13 | 0.76     | 1.57        | 1      | 4     |
| 1:B:109:LEU:HD22 | 1:B:157:LEU:HD22 | 0.74     | 1.59        | 8      | 9     |
| 1:A:99:LEU:HD23  | 1:A:140:ARG:NE   | 0.74     | 1.97        | 7      | 2     |
| 1:B:102:ASN:CB   | 1:B:109:LEU:HD13 | 0.73     | 2.14        | 5      | 8     |
| 1:A:102:ASN:HB2  | 1:A:109:LEU:HD13 | 0.71     | 1.61        | 9      | 2     |
| 1:A:109:LEU:HD22 | 1:A:157:LEU:HD22 | 0.70     | 1.61        | 2      | 10    |
| 1:A:99:LEU:HD22  | 1:A:120:ILE:HG13 | 0.69     | 1.62        | 2      | 1     |
| 1:B:102:ASN:HB2  | 1:B:109:LEU:HD13 | 0.69     | 1.63        | 2      | 3     |
| 1:A:127:ARG:CZ   | 1:A:127:ARG:HB3  | 0.69     | 2.16        | 2      | 3     |
| 1:A:119:GLU:CD   | 1:A:141:LYS:NZ   | 0.69     | 2.51        | 1      | 2     |
| 1:B:99:LEU:HD22  | 1:B:120:ILE:HG13 | 0.68     | 1.65        | 3      | 1     |
| 1:A:117:VAL:HG22 | 1:A:143:THR:HG23 | 0.68     | 1.66        | 8      | 4     |
| 1:A:140:ARG:NH2  | 1:A:142:TYR:CD1  | 0.68     | 2.62        | 8      | 1     |
| 1:B:95:TRP:NE1   | 1:B:97:VAL:HG22  | 0.67     | 2.04        | 1      | 2     |
| 1:A:152:GLN:O    | 1:A:167:ALA:HB1  | 0.67     | 1.89        | 2      | 8     |
| 1:A:140:ARG:NH2  | 1:A:142:TYR:CE1  | 0.67     | 2.62        | 8      | 1     |
| 1:B:102:ASN:ND2  | 1:B:102:ASN:H    | 0.66     | 1.88        | 9      | 2     |
| 1:A:153:VAL:HG22 | 1:A:169:MET:HE1  | 0.66     | 1.68        | 3      | 1     |
| 1:A:101:VAL:HG11 | 1:A:138:PHE:CD2  | 0.65     | 2.27        | 7      | 3     |
| 1:A:148:VAL:HA   | 1:A:169:MET:SD   | 0.65     | 2.31        | 3      | 2     |
| 1:A:119:GLU:CD   | 1:A:141:LYS:HZ2  | 0.65     | 1.99        | 7      | 1     |
| 1:B:102:ASN:OD1  | 1:B:157:LEU:HD11 | 0.65     | 1.91        | 5      | 3     |
| 1:A:153:VAL:CG2  | 1:A:169:MET:HE1  | 0.65     | 2.21        | 3      | 1     |
| 1:A:95:TRP:CZ3   | 1:A:97:VAL:HG21  | 0.64     | 2.27        | 9      | 4     |
| 1:B:130:GLU:N    | 1:B:130:GLU:CD   | 0.64     | 2.56        | 10     | 1     |
| 1:A:127:ARG:CZ   | 1:A:127:ARG:CB   | 0.63     | 2.76        | 2      | 2     |
| 1:B:109:LEU:CD2  | 1:B:157:LEU:HD22 | 0.63     | 2.23        | 8      | 4     |
| 1:B:163:LEU:C    | 1:B:163:LEU:HD13 | 0.63     | 2.18        | 2      | 10    |
| 1:B:102:ASN:OD1  | 1:B:109:LEU:HD13 | 0.63     | 1.92        | 6      | 3     |
| 1:A:102:ASN:CB   | 1:A:109:LEU:HD13 | 0.63     | 2.24        | 1      | 7     |
| 1:A:109:LEU:CD2  | 1:A:157:LEU:HD22 | 0.62     | 2.25        | 7      | 5     |
| 1:A:102:ASN:ND2  | 1:A:102:ASN:H    | 0.62     | 1.92        | 1      | 2     |
| 1:B:95:TRP:HB2   | 1:B:169:MET:SD   | 0.61     | 2.35        | 4      | 3     |
| 1:B:124:HIS:H    | 1:B:124:HIS:CD2  | 0.61     | 2.13        | 8      | 1     |
| 1:B:114:LYS:O    | 1:B:116:GLY:N    | 0.61     | 2.33        | 5      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:102:ASN:OD1  | 1:B:161:GLY:HA2  | 0.61     | 1.95        | 5      | 3     |
| 1:A:125:GLU:O    | 1:A:126:GLU:C    | 0.61     | 2.44        | 10     | 8     |
| 1:B:169:MET:SD   | 1:B:169:MET:N    | 0.60     | 2.74        | 7      | 2     |
| 1:A:99:LEU:HD22  | 1:A:120:ILE:HG12 | 0.60     | 1.73        | 7      | 4     |
| 1:A:163:LEU:C    | 1:A:163:LEU:HD13 | 0.60     | 2.22        | 2      | 10    |
| 1:A:166:GLU:O    | 1:A:167:ALA:HB2  | 0.60     | 1.95        | 1      | 7     |
| 1:A:102:ASN:OD1  | 1:A:109:LEU:HD13 | 0.60     | 1.96        | 7      | 6     |
| 1:A:142:TYR:CE1  | 1:B:132:GLY:HA3  | 0.60     | 2.32        | 9      | 2     |
| 1:B:125:GLU:O    | 1:B:126:GLU:C    | 0.60     | 2.45        | 7      | 8     |
| 1:A:99:LEU:HD22  | 1:A:120:ILE:CG1  | 0.60     | 2.27        | 4      | 3     |
| 1:B:102:ASN:ND2  | 1:B:102:ASN:N    | 0.59     | 2.48        | 9      | 2     |
| 1:B:140:ARG:NH1  | 1:B:142:TYR:OH   | 0.59     | 2.30        | 8      | 1     |
| 1:B:102:ASN:ND2  | 1:B:161:GLY:O    | 0.59     | 2.35        | 9      | 4     |
| 1:B:114:LYS:O    | 1:B:117:VAL:N    | 0.59     | 2.34        | 5      | 3     |
| 1:B:99:LEU:HD22  | 1:B:120:ILE:CG1  | 0.59     | 2.28        | 2      | 4     |
| 1:A:95:TRP:NE1   | 1:A:97:VAL:CG2   | 0.59     | 2.65        | 7      | 2     |
| 1:B:108:GLU:CD   | 1:B:123:LYS:HZ3  | 0.59     | 2.06        | 5      | 1     |
| 1:B:152:GLN:O    | 1:B:167:ALA:HB1  | 0.59     | 1.96        | 9      | 3     |
| 1:A:95:TRP:NE1   | 1:A:97:VAL:HG22  | 0.59     | 2.13        | 10     | 2     |
| 1:A:134:ILE:O    | 1:A:136:ARG:NH2  | 0.59     | 2.35        | 4      | 1     |
| 1:B:99:LEU:HD23  | 1:B:140:ARG:NE   | 0.58     | 2.12        | 4      | 1     |
| 1:B:108:GLU:CD   | 1:B:123:LYS:NZ   | 0.58     | 2.61        | 5      | 2     |
| 1:A:158:SER:O    | 1:A:161:GLY:N    | 0.58     | 2.36        | 4      | 2     |
| 1:B:99:LEU:HD23  | 1:B:140:ARG:HH11 | 0.58     | 1.59        | 8      | 1     |
| 1:A:95:TRP:C     | 1:A:95:TRP:CD1   | 0.58     | 2.81        | 1      | 2     |
| 1:B:99:LEU:HD21  | 1:B:142:TYR:CE1  | 0.58     | 2.33        | 9      | 1     |
| 1:A:140:ARG:NH2  | 1:A:142:TYR:OH   | 0.58     | 2.34        | 7      | 4     |
| 1:B:145:PRO:O    | 1:B:147:GLY:N    | 0.58     | 2.37        | 10     | 9     |
| 1:A:134:ILE:HD12 | 1:B:140:ARG:NH1  | 0.58     | 2.14        | 2      | 1     |
| 1:B:102:ASN:C    | 1:B:102:ASN:ND2  | 0.58     | 2.62        | 10     | 1     |
| 1:A:100:ASP:C    | 1:A:101:VAL:HG22 | 0.58     | 2.23        | 9      | 3     |
| 1:A:102:ASN:ND2  | 1:A:102:ASN:N    | 0.58     | 2.50        | 1      | 2     |
| 1:A:132:GLY:HA3  | 1:B:142:TYR:CE1  | 0.58     | 2.33        | 2      | 1     |
| 1:A:114:LYS:O    | 1:A:116:GLY:N    | 0.58     | 2.36        | 9      | 1     |
| 1:B:102:ASN:C    | 1:B:102:ASN:HD22 | 0.58     | 2.07        | 10     | 2     |
| 1:B:102:ASN:ND2  | 1:B:105:ALA:O    | 0.58     | 2.34        | 3      | 2     |
| 1:A:145:PRO:CD   | 1:A:146:PRO:HD3  | 0.57     | 2.29        | 1      | 10    |
| 1:A:102:ASN:O    | 1:A:102:ASN:ND2  | 0.57     | 2.34        | 9      | 3     |
| 1:A:99:LEU:HD23  | 1:A:140:ARG:HE   | 0.57     | 1.60        | 7      | 1     |
| 1:B:102:ASN:OD1  | 1:B:109:LEU:CD1  | 0.57     | 2.52        | 6      | 2     |
| 1:A:95:TRP:CH2   | 1:A:148:VAL:HG21 | 0.57     | 2.35        | 2      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:112:LYS:NZ   | 1:A:119:GLU:HB2  | 0.57     | 2.14        | 9      | 1     |
| 1:A:165:VAL:O    | 1:A:165:VAL:HG23 | 0.57     | 1.99        | 7      | 10    |
| 1:B:129:ASP:CG   | 1:B:130:GLU:N    | 0.57     | 2.62        | 10     | 5     |
| 1:A:140:ARG:NE   | 1:A:142:TYR:OH   | 0.57     | 2.35        | 4      | 1     |
| 1:A:127:ARG:CB   | 1:A:127:ARG:NH1  | 0.57     | 2.68        | 2      | 2     |
| 1:A:145:PRO:HD2  | 1:A:146:PRO:CD   | 0.57     | 2.30        | 6      | 1     |
| 1:A:95:TRP:CB    | 1:A:169:MET:SD   | 0.57     | 2.93        | 5      | 1     |
| 1:A:102:ASN:HD22 | 1:A:102:ASN:C    | 0.56     | 2.08        | 6      | 1     |
| 1:A:102:ASN:ND2  | 1:A:161:GLY:O    | 0.56     | 2.37        | 1      | 5     |
| 1:B:102:ASN:O    | 1:B:102:ASN:ND2  | 0.56     | 2.37        | 2      | 3     |
| 1:B:145:PRO:HD2  | 1:B:146:PRO:CD   | 0.56     | 2.30        | 5      | 7     |
| 1:B:108:GLU:OE1  | 1:B:123:LYS:NZ   | 0.56     | 2.37        | 3      | 4     |
| 1:A:102:ASN:OD1  | 1:A:161:GLY:HA2  | 0.56     | 2.00        | 8      | 2     |
| 1:A:119:GLU:CD   | 1:A:141:LYS:HZ3  | 0.56     | 2.07        | 1      | 1     |
| 1:B:145:PRO:N    | 1:B:146:PRO:CD   | 0.56     | 2.68        | 1      | 9     |
| 1:A:140:ARG:NH1  | 1:A:142:TYR:OH   | 0.56     | 2.34        | 2      | 2     |
| 1:A:102:ASN:CG   | 1:A:109:LEU:HD13 | 0.56     | 2.25        | 5      | 6     |
| 1:A:158:SER:HB2  | 1:A:162:THR:HG22 | 0.56     | 1.77        | 4      | 1     |
| 1:B:95:TRP:NE1   | 1:B:97:VAL:CG2   | 0.56     | 2.68        | 8      | 2     |
| 1:B:102:ASN:CG   | 1:B:109:LEU:HD13 | 0.56     | 2.25        | 6      | 5     |
| 1:A:102:ASN:OD1  | 1:A:109:LEU:HD22 | 0.56     | 1.99        | 6      | 2     |
| 1:A:145:PRO:HD2  | 1:A:146:PRO:HD3  | 0.56     | 1.78        | 9      | 10    |
| 1:A:102:ASN:OD1  | 1:A:157:LEU:HD11 | 0.56     | 1.99        | 8      | 2     |
| 1:A:159:PRO:C    | 1:A:161:GLY:H    | 0.56     | 2.09        | 9      | 4     |
| 1:A:140:ARG:NH1  | 1:B:133:TYR:O    | 0.55     | 2.29        | 8      | 1     |
| 1:B:145:PRO:N    | 1:B:146:PRO:HD2  | 0.55     | 2.16        | 2      | 8     |
| 1:B:102:ASN:ND2  | 1:B:102:ASN:C    | 0.55     | 2.64        | 2      | 1     |
| 1:A:134:ILE:HD13 | 1:A:136:ARG:NH2  | 0.55     | 2.16        | 6      | 2     |
| 1:B:101:VAL:C    | 1:B:103:HIS:H    | 0.55     | 2.08        | 6      | 3     |
| 1:A:95:TRP:CZ2   | 1:A:148:VAL:CG2  | 0.55     | 2.89        | 1      | 2     |
| 1:A:99:LEU:CD2   | 1:A:140:ARG:HB3  | 0.55     | 2.31        | 8      | 1     |
| 1:A:140:ARG:NH2  | 1:A:141:LYS:C    | 0.55     | 2.65        | 8      | 1     |
| 1:B:159:PRO:C    | 1:B:161:GLY:H    | 0.55     | 2.09        | 2      | 7     |
| 1:B:127:ARG:HB2  | 1:B:127:ARG:NH1  | 0.55     | 2.17        | 7      | 1     |
| 1:B:100:ASP:C    | 1:B:101:VAL:HG22 | 0.54     | 2.26        | 1      | 6     |
| 1:A:108:GLU:OE1  | 1:A:123:LYS:NZ   | 0.54     | 2.38        | 3      | 1     |
| 1:B:126:GLU:HA   | 1:B:135:SER:OG   | 0.54     | 2.02        | 1      | 6     |
| 1:B:99:LEU:O     | 1:B:140:ARG:NH2  | 0.54     | 2.32        | 3      | 2     |
| 1:A:112:LYS:NZ   | 1:A:119:GLU:CB   | 0.54     | 2.70        | 9      | 2     |
| 1:B:168:PRO:C    | 1:B:169:MET:HG3  | 0.54     | 2.28        | 6      | 1     |
| 1:A:114:LYS:O    | 1:A:117:VAL:HG23 | 0.54     | 2.03        | 5      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:102:ASN:OD1  | 1:B:157:LEU:CD1  | 0.54     | 2.55        | 5      | 1     |
| 1:A:119:GLU:CD   | 1:A:141:LYS:HD3  | 0.54     | 2.27        | 10     | 1     |
| 1:B:95:TRP:CZ3   | 1:B:97:VAL:HG21  | 0.54     | 2.38        | 6      | 1     |
| 1:B:114:LYS:NZ   | 1:B:119:GLU:OE2  | 0.54     | 2.39        | 2      | 5     |
| 1:A:124:HIS:ND1  | 1:A:125:GLU:N    | 0.54     | 2.56        | 6      | 1     |
| 1:B:145:PRO:CD   | 1:B:146:PRO:CD   | 0.54     | 2.85        | 5      | 6     |
| 1:B:165:VAL:O    | 1:B:165:VAL:HG23 | 0.54     | 2.02        | 1      | 10    |
| 1:A:102:ASN:HD22 | 1:A:102:ASN:H    | 0.54     | 1.46        | 3      | 1     |
| 1:B:114:LYS:CB   | 1:B:114:LYS:NZ   | 0.54     | 2.71        | 8      | 1     |
| 1:A:102:ASN:ND2  | 1:A:161:GLY:C    | 0.53     | 2.66        | 1      | 2     |
| 1:B:149:ASP:O    | 1:B:153:VAL:HG23 | 0.53     | 2.03        | 7      | 6     |
| 1:A:142:TYR:CZ   | 1:B:131:HIS:O    | 0.53     | 2.61        | 2      | 6     |
| 1:B:112:LYS:NZ   | 1:B:121:THR:OG1  | 0.53     | 2.40        | 5      | 2     |
| 1:B:148:VAL:CG1  | 1:B:148:VAL:O    | 0.53     | 2.56        | 10     | 3     |
| 1:A:142:TYR:CE1  | 1:B:131:HIS:O    | 0.53     | 2.61        | 8      | 2     |
| 1:A:102:ASN:OD1  | 1:A:109:LEU:CD1  | 0.53     | 2.56        | 7      | 3     |
| 1:B:145:PRO:CD   | 1:B:146:PRO:HD3  | 0.53     | 2.34        | 9      | 4     |
| 1:A:95:TRP:HB3   | 1:A:169:MET:SD   | 0.53     | 2.43        | 10     | 1     |
| 1:B:119:GLU:C    | 1:B:120:ILE:HD13 | 0.53     | 2.28        | 6      | 2     |
| 1:B:136:ARG:HD3  | 1:B:138:PHE:CE1  | 0.53     | 2.39        | 8      | 1     |
| 1:A:102:ASN:O    | 1:A:105:ALA:N    | 0.52     | 2.40        | 6      | 2     |
| 1:A:101:VAL:C    | 1:A:103:HIS:H    | 0.52     | 2.11        | 7      | 6     |
| 1:B:119:GLU:HG2  | 1:B:141:LYS:HA   | 0.52     | 1.82        | 6      | 2     |
| 1:A:134:ILE:CD1  | 1:A:136:ARG:NH2  | 0.52     | 2.72        | 6      | 1     |
| 1:B:102:ASN:HD21 | 1:B:105:ALA:C    | 0.52     | 2.12        | 3      | 1     |
| 1:B:96:ARG:NH1   | 1:B:96:ARG:HB2   | 0.52     | 2.19        | 4      | 1     |
| 1:B:115:ASP:O    | 1:B:115:ASP:CG   | 0.52     | 2.50        | 4      | 1     |
| 1:A:115:ASP:O    | 1:A:115:ASP:CG   | 0.52     | 2.50        | 5      | 2     |
| 1:A:101:VAL:HG11 | 1:A:138:PHE:CD1  | 0.52     | 2.40        | 1      | 1     |
| 1:B:156:SER:O    | 1:B:163:LEU:HD22 | 0.52     | 2.04        | 3      | 4     |
| 1:B:145:PRO:C    | 1:B:147:GLY:N    | 0.52     | 2.67        | 7      | 7     |
| 1:B:163:LEU:C    | 1:B:163:LEU:CD1  | 0.52     | 2.83        | 1      | 10    |
| 1:A:142:TYR:OH   | 1:B:131:HIS:O    | 0.52     | 2.26        | 7      | 2     |
| 1:A:127:ARG:NH1  | 1:A:127:ARG:HB2  | 0.52     | 2.19        | 2      | 2     |
| 1:B:104:PHE:HB2  | 1:B:124:HIS:CE1  | 0.52     | 2.40        | 2      | 1     |
| 1:B:108:GLU:OE2  | 1:B:123:LYS:NZ   | 0.52     | 2.41        | 4      | 4     |
| 1:A:112:LYS:NZ   | 1:A:121:THR:OG1  | 0.52     | 2.35        | 10     | 5     |
| 1:A:101:VAL:O    | 1:A:103:HIS:N    | 0.52     | 2.42        | 7      | 5     |
| 1:B:94:ARG:NH1   | 1:B:166:GLU:OE1  | 0.52     | 2.42        | 2      | 3     |
| 1:A:95:TRP:CH2   | 1:A:148:VAL:CG2  | 0.52     | 2.93        | 9      | 3     |
| 1:B:124:HIS:O    | 1:B:135:SER:CB   | 0.52     | 2.58        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:127:ARG:CB   | 1:B:127:ARG:CZ   | 0.52     | 2.88        | 7      | 1     |
| 1:B:153:VAL:HA   | 1:B:167:ALA:HB2  | 0.51     | 1.82        | 10     | 5     |
| 1:A:114:LYS:O    | 1:A:117:VAL:N    | 0.51     | 2.34        | 5      | 1     |
| 1:B:94:ARG:HH12  | 1:B:166:GLU:CD   | 0.51     | 2.14        | 1      | 1     |
| 1:B:142:TYR:CD1  | 1:B:142:TYR:N    | 0.51     | 2.78        | 9      | 5     |
| 1:B:102:ASN:CG   | 1:B:161:GLY:HA2  | 0.51     | 2.30        | 5      | 3     |
| 1:B:140:ARG:HB3  | 1:B:140:ARG:CZ   | 0.51     | 2.34        | 8      | 1     |
| 1:B:102:ASN:N    | 1:B:102:ASN:HD22 | 0.51     | 2.03        | 1      | 2     |
| 1:A:158:SER:HB3  | 1:A:162:THR:OG1  | 0.51     | 2.05        | 2      | 1     |
| 1:B:145:PRO:HD2  | 1:B:146:PRO:HD3  | 0.51     | 1.83        | 9      | 6     |
| 1:A:127:ARG:N    | 1:A:135:SER:OG   | 0.51     | 2.44        | 6      | 1     |
| 1:A:169:MET:HE3  | 1:A:169:MET:H    | 0.51     | 1.64        | 9      | 1     |
| 1:B:119:GLU:CD   | 1:B:141:LYS:HZ2  | 0.51     | 2.14        | 9      | 1     |
| 1:B:100:ASP:C    | 1:B:101:VAL:CG2  | 0.51     | 2.84        | 4      | 7     |
| 1:B:143:THR:O    | 1:B:145:PRO:HD3  | 0.51     | 2.05        | 1      | 8     |
| 1:B:153:VAL:HG22 | 1:B:167:ALA:CB   | 0.51     | 2.36        | 4      | 5     |
| 1:A:167:ALA:HB1  | 1:A:168:PRO:HD2  | 0.50     | 1.83        | 1      | 7     |
| 1:A:114:LYS:NZ   | 1:A:119:GLU:OE1  | 0.50     | 2.42        | 5      | 3     |
| 1:B:95:TRP:CD1   | 1:B:169:MET:HE3  | 0.50     | 2.41        | 8      | 1     |
| 1:B:102:ASN:O    | 1:B:104:PHE:N    | 0.50     | 2.44        | 3      | 1     |
| 1:B:107:ASP:C    | 1:B:109:LEU:H    | 0.50     | 2.14        | 2      | 1     |
| 1:A:95:TRP:HB2   | 1:A:169:MET:SD   | 0.50     | 2.46        | 5      | 1     |
| 1:B:95:TRP:C     | 1:B:95:TRP:CD1   | 0.50     | 2.90        | 6      | 1     |
| 1:A:141:LYS:NZ   | 1:B:126:GLU:OE1  | 0.50     | 2.41        | 5      | 2     |
| 1:A:126:GLU:OE1  | 1:B:141:LYS:NZ   | 0.50     | 2.43        | 7      | 3     |
| 1:B:148:VAL:O    | 1:B:148:VAL:CG1  | 0.50     | 2.59        | 2      | 2     |
| 1:B:134:ILE:O    | 1:B:136:ARG:NH2  | 0.50     | 2.36        | 3      | 1     |
| 1:A:108:GLU:N    | 1:A:108:GLU:CD   | 0.50     | 2.69        | 7      | 1     |
| 1:A:167:ALA:HB3  | 1:A:169:MET:SD   | 0.50     | 2.47        | 8      | 1     |
| 1:A:140:ARG:HA   | 1:A:140:ARG:NH1  | 0.50     | 2.22        | 10     | 1     |
| 1:A:101:VAL:HA   | 1:A:103:HIS:CE1  | 0.50     | 2.42        | 9      | 2     |
| 1:A:165:VAL:O    | 1:A:165:VAL:CG2  | 0.49     | 2.59        | 4      | 9     |
| 1:B:101:VAL:O    | 1:B:103:HIS:N    | 0.49     | 2.45        | 6      | 2     |
| 1:B:102:ASN:ND2  | 1:B:161:GLY:C    | 0.49     | 2.70        | 9      | 2     |
| 1:B:149:ASP:O    | 1:B:153:VAL:CG2  | 0.49     | 2.60        | 7      | 4     |
| 1:A:108:GLU:OE2  | 1:A:123:LYS:NZ   | 0.49     | 2.42        | 8      | 3     |
| 1:B:127:ARG:NH1  | 1:B:135:SER:HA   | 0.49     | 2.22        | 9      | 1     |
| 1:A:157:LEU:HD12 | 1:A:158:SER:N    | 0.49     | 2.22        | 3      | 1     |
| 1:B:140:ARG:NH2  | 1:B:142:TYR:OH   | 0.49     | 2.37        | 7      | 3     |
| 1:A:166:GLU:CD   | 1:A:166:GLU:C    | 0.49     | 2.79        | 7      | 3     |
| 1:B:114:LYS:NZ   | 1:B:115:ASP:OD1  | 0.49     | 2.45        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:104:PHE:O    | 1:A:124:HIS:ND1  | 0.49     | 2.34        | 1      | 2     |
| 1:A:101:VAL:HG11 | 1:A:138:PHE:CE2  | 0.49     | 2.42        | 7      | 1     |
| 1:A:95:TRP:CH2   | 1:A:97:VAL:HG21  | 0.49     | 2.42        | 1      | 1     |
| 1:B:102:ASN:C    | 1:B:104:PHE:N    | 0.49     | 2.69        | 5      | 3     |
| 1:A:163:LEU:C    | 1:A:163:LEU:CD1  | 0.49     | 2.85        | 4      | 10    |
| 1:A:169:MET:CB   | 1:A:170:PRO:CD   | 0.49     | 2.91        | 7      | 1     |
| 1:B:102:ASN:O    | 1:B:105:ALA:N    | 0.49     | 2.39        | 7      | 3     |
| 1:A:153:VAL:HA   | 1:A:167:ALA:HB2  | 0.49     | 1.84        | 5      | 1     |
| 1:A:101:VAL:HG21 | 1:A:138:PHE:CD2  | 0.49     | 2.43        | 8      | 1     |
| 1:A:103:HIS:N    | 1:A:161:GLY:HA3  | 0.49     | 2.23        | 10     | 2     |
| 1:A:95:TRP:CD1   | 1:A:95:TRP:C     | 0.49     | 2.91        | 6      | 2     |
| 1:B:101:VAL:CG2  | 1:B:140:ARG:CZ   | 0.49     | 2.91        | 4      | 1     |
| 1:A:101:VAL:CG1  | 1:A:138:PHE:CD2  | 0.49     | 2.96        | 9      | 2     |
| 1:A:145:PRO:CD   | 1:A:146:PRO:CD   | 0.48     | 2.90        | 6      | 1     |
| 1:B:94:ARG:NH2   | 1:B:166:GLU:OE2  | 0.48     | 2.40        | 8      | 1     |
| 1:A:142:TYR:CD1  | 1:A:142:TYR:N    | 0.48     | 2.80        | 1      | 3     |
| 1:A:95:TRP:CG    | 1:A:96:ARG:N     | 0.48     | 2.81        | 10     | 1     |
| 1:A:114:LYS:NZ   | 1:A:119:GLU:OE2  | 0.48     | 2.43        | 10     | 2     |
| 1:A:102:ASN:N    | 1:A:102:ASN:HD22 | 0.48     | 2.06        | 5      | 2     |
| 1:A:145:PRO:CB   | 1:A:146:PRO:HD3  | 0.48     | 2.39        | 1      | 9     |
| 1:B:100:ASP:O    | 1:B:101:VAL:HG22 | 0.48     | 2.08        | 4      | 1     |
| 1:B:158:SER:O    | 1:B:161:GLY:N    | 0.48     | 2.45        | 10     | 3     |
| 1:A:134:ILE:HD13 | 1:A:136:ARG:HH21 | 0.48     | 1.69        | 4      | 1     |
| 1:B:107:ASP:OD1  | 1:B:107:ASP:N    | 0.48     | 2.46        | 6      | 1     |
| 1:A:166:GLU:O    | 1:A:167:ALA:CB   | 0.48     | 2.62        | 1      | 3     |
| 1:A:136:ARG:NH1  | 1:B:138:PHE:CZ   | 0.48     | 2.82        | 2      | 1     |
| 1:B:128:GLN:HG2  | 1:B:129:ASP:N    | 0.48     | 2.24        | 6      | 1     |
| 1:B:104:PHE:O    | 1:B:136:ARG:NH2  | 0.48     | 2.43        | 10     | 1     |
| 1:B:114:LYS:NZ   | 1:B:119:GLU:OE1  | 0.48     | 2.41        | 10     | 1     |
| 1:A:126:GLU:OE2  | 1:B:141:LYS:NZ   | 0.47     | 2.42        | 10     | 4     |
| 1:B:136:ARG:CZ   | 1:B:138:PHE:CZ   | 0.47     | 2.97        | 4      | 1     |
| 1:B:124:HIS:ND1  | 1:B:126:GLU:O    | 0.47     | 2.43        | 9      | 1     |
| 1:A:141:LYS:NZ   | 1:B:126:GLU:OE2  | 0.47     | 2.41        | 9      | 2     |
| 1:B:95:TRP:CB    | 1:B:169:MET:SD   | 0.47     | 3.02        | 4      | 2     |
| 1:A:101:VAL:C    | 1:A:103:HIS:N    | 0.47     | 2.70        | 6      | 5     |
| 1:B:166:GLU:O    | 1:B:167:ALA:HB2  | 0.47     | 2.10        | 1      | 1     |
| 1:B:134:ILE:O    | 1:B:134:ILE:HG23 | 0.47     | 2.09        | 2      | 4     |
| 1:B:102:ASN:ND2  | 1:B:102:ASN:O    | 0.47     | 2.47        | 10     | 2     |
| 1:A:153:VAL:HG22 | 1:A:167:ALA:CB   | 0.47     | 2.40        | 5      | 1     |
| 1:B:168:PRO:O    | 1:B:169:MET:O    | 0.47     | 2.33        | 6      | 1     |
| 1:B:109:LEU:HD22 | 1:B:157:LEU:CD2  | 0.47     | 2.36        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:101:VAL:N    | 1:B:103:HIS:CE1  | 0.47     | 2.83        | 1      | 1     |
| 1:B:160:GLU:H    | 1:B:160:GLU:CD   | 0.47     | 2.18        | 1      | 1     |
| 1:B:165:VAL:O    | 1:B:165:VAL:CG2  | 0.47     | 2.63        | 1      | 9     |
| 1:B:166:GLU:CD   | 1:B:166:GLU:C    | 0.47     | 2.83        | 4      | 2     |
| 1:A:100:ASP:OD1  | 1:A:140:ARG:NH2  | 0.47     | 2.44        | 6      | 1     |
| 1:B:127:ARG:NH2  | 1:B:136:ARG:O    | 0.47     | 2.47        | 9      | 1     |
| 1:A:117:VAL:HG13 | 1:A:143:THR:HG23 | 0.46     | 1.86        | 9      | 2     |
| 1:A:134:ILE:HD11 | 1:A:136:ARG:HH11 | 0.46     | 1.68        | 8      | 1     |
| 1:A:140:ARG:HH22 | 1:A:141:LYS:C    | 0.46     | 2.18        | 8      | 1     |
| 1:B:124:HIS:CD2  | 1:B:136:ARG:H    | 0.46     | 2.27        | 8      | 1     |
| 1:A:124:HIS:ND1  | 1:A:127:ARG:HG2  | 0.46     | 2.26        | 9      | 2     |
| 1:B:145:PRO:C    | 1:B:147:GLY:H    | 0.46     | 2.18        | 3      | 6     |
| 1:B:101:VAL:C    | 1:B:103:HIS:N    | 0.46     | 2.73        | 6      | 4     |
| 1:A:112:LYS:NZ   | 1:A:119:GLU:OE1  | 0.46     | 2.49        | 9      | 1     |
| 1:A:99:LEU:HD22  | 1:A:120:ILE:HB   | 0.46     | 1.86        | 8      | 1     |
| 1:B:119:GLU:O    | 1:B:120:ILE:HD12 | 0.46     | 2.11        | 9      | 2     |
| 1:B:102:ASN:CG   | 1:B:102:ASN:O    | 0.46     | 2.58        | 3      | 1     |
| 1:B:109:LEU:HD11 | 1:B:120:ILE:HG23 | 0.46     | 1.88        | 1      | 1     |
| 1:B:148:VAL:O    | 1:B:149:ASP:C    | 0.46     | 2.59        | 3      | 1     |
| 1:A:112:LYS:HZ3  | 1:A:119:GLU:HB2  | 0.46     | 1.68        | 9      | 1     |
| 1:A:117:VAL:HG22 | 1:A:143:THR:CG2  | 0.46     | 2.41        | 10     | 1     |
| 1:A:114:LYS:O    | 1:A:115:ASP:C    | 0.46     | 2.59        | 4      | 5     |
| 1:A:140:ARG:CZ   | 1:A:142:TYR:CZ   | 0.46     | 2.99        | 8      | 1     |
| 1:A:123:LYS:O    | 1:A:123:LYS:NZ   | 0.46     | 2.35        | 9      | 1     |
| 1:B:124:HIS:CD2  | 1:B:127:ARG:CZ   | 0.46     | 2.99        | 10     | 1     |
| 1:B:114:LYS:O    | 1:B:115:ASP:C    | 0.46     | 2.59        | 1      | 7     |
| 1:A:95:TRP:CZ3   | 1:A:97:VAL:CG2   | 0.46     | 2.99        | 2      | 3     |
| 1:A:109:LEU:HD22 | 1:A:157:LEU:CD2  | 0.46     | 2.35        | 2      | 3     |
| 1:B:145:PRO:CB   | 1:B:146:PRO:HD3  | 0.46     | 2.41        | 9      | 1     |
| 1:B:95:TRP:CD1   | 1:B:97:VAL:HG22  | 0.46     | 2.46        | 1      | 1     |
| 1:B:100:ASP:CG   | 1:B:103:HIS:HE2  | 0.46     | 2.19        | 2      | 1     |
| 1:B:160:GLU:N    | 1:B:160:GLU:CD   | 0.46     | 2.74        | 9      | 1     |
| 1:A:94:ARG:NH1   | 1:A:166:GLU:OE1  | 0.45     | 2.49        | 9      | 2     |
| 1:B:149:ASP:OD1  | 1:B:152:GLN:N    | 0.45     | 2.45        | 2      | 1     |
| 1:B:134:ILE:HD11 | 1:B:136:ARG:NH2  | 0.45     | 2.25        | 7      | 1     |
| 1:A:102:ASN:CB   | 1:A:109:LEU:CD1  | 0.45     | 2.94        | 10     | 1     |
| 1:B:124:HIS:O    | 1:B:135:SER:HB3  | 0.45     | 2.11        | 4      | 2     |
| 1:B:112:LYS:NZ   | 1:B:119:GLU:HB2  | 0.45     | 2.25        | 1      | 1     |
| 1:A:100:ASP:C    | 1:A:101:VAL:CG2  | 0.45     | 2.88        | 9      | 5     |
| 1:A:162:THR:O    | 1:A:162:THR:CG2  | 0.45     | 2.65        | 4      | 1     |
| 1:A:95:TRP:HE1   | 1:A:97:VAL:HG22  | 0.45     | 1.71        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:102:ASN:ND2  | 1:B:161:GLY:CA   | 0.45     | 2.79        | 1      | 2     |
| 1:B:111:VAL:HG13 | 1:B:120:ILE:CD1  | 0.45     | 2.42        | 2      | 1     |
| 1:B:109:LEU:HA   | 1:B:121:THR:O    | 0.45     | 2.11        | 8      | 2     |
| 1:B:102:ASN:HB3  | 1:B:109:LEU:CD1  | 0.45     | 2.41        | 7      | 1     |
| 1:A:169:MET:SD   | 1:A:169:MET:N    | 0.45     | 2.90        | 1      | 1     |
| 1:A:125:GLU:O    | 1:A:126:GLU:HB2  | 0.45     | 2.12        | 9      | 2     |
| 1:A:126:GLU:HA   | 1:A:135:SER:OG   | 0.45     | 2.12        | 4      | 4     |
| 1:A:158:SER:C    | 1:A:160:GLU:N    | 0.45     | 2.74        | 2      | 1     |
| 1:B:109:LEU:HG   | 1:B:110:THR:N    | 0.45     | 2.27        | 6      | 2     |
| 1:A:119:GLU:HA   | 1:A:140:ARG:O    | 0.45     | 2.12        | 8      | 1     |
| 1:B:124:HIS:NE2  | 1:B:136:ARG:HG3  | 0.45     | 2.27        | 8      | 1     |
| 1:B:144:LEU:C    | 1:B:146:PRO:HD2  | 0.45     | 2.37        | 2      | 1     |
| 1:B:98:SER:HA    | 1:B:163:LEU:O    | 0.45     | 2.11        | 8      | 3     |
| 1:B:108:GLU:CD   | 1:B:123:LYS:HZ1  | 0.45     | 2.19        | 4      | 1     |
| 1:A:125:GLU:O    | 1:A:127:ARG:N    | 0.45     | 2.50        | 3      | 1     |
| 1:A:167:ALA:HB3  | 1:A:169:MET:HE3  | 0.45     | 1.89        | 3      | 1     |
| 1:B:119:GLU:O    | 1:B:120:ILE:HD13 | 0.45     | 2.12        | 6      | 1     |
| 1:B:157:LEU:HD12 | 1:B:158:SER:N    | 0.45     | 2.27        | 1      | 1     |
| 1:A:99:LEU:HD23  | 1:A:140:ARG:HG3  | 0.45     | 1.89        | 2      | 1     |
| 1:B:104:PHE:O    | 1:B:124:HIS:ND1  | 0.45     | 2.34        | 5      | 2     |
| 1:B:159:PRO:C    | 1:B:161:GLY:N    | 0.44     | 2.76        | 2      | 7     |
| 1:B:111:VAL:HG13 | 1:B:120:ILE:HD12 | 0.44     | 1.89        | 5      | 1     |
| 1:B:103:HIS:N    | 1:B:161:GLY:HA3  | 0.44     | 2.28        | 7      | 2     |
| 1:A:169:MET:HB3  | 1:A:170:PRO:HD2  | 0.44     | 1.90        | 8      | 1     |
| 1:A:162:THR:HG23 | 1:A:162:THR:O    | 0.44     | 2.12        | 10     | 1     |
| 1:A:167:ALA:HB3  | 1:A:169:MET:CE   | 0.44     | 2.42        | 3      | 1     |
| 1:B:168:PRO:C    | 1:B:169:MET:CG   | 0.44     | 2.90        | 4      | 1     |
| 1:A:159:PRO:C    | 1:A:161:GLY:N    | 0.44     | 2.76        | 7      | 4     |
| 1:A:102:ASN:CG   | 1:A:161:GLY:HA2  | 0.44     | 2.37        | 8      | 2     |
| 1:A:136:ARG:NH1  | 1:B:138:PHE:CE2  | 0.44     | 2.85        | 9      | 1     |
| 1:A:149:ASP:OD1  | 1:A:151:THR:N    | 0.44     | 2.51        | 9      | 2     |
| 1:B:149:ASP:CG   | 1:B:152:GLN:HG3  | 0.44     | 2.38        | 10     | 1     |
| 1:B:99:LEU:CD2   | 1:B:140:ARG:HB2  | 0.44     | 2.42        | 4      | 1     |
| 1:B:123:LYS:C    | 1:B:124:HIS:ND1  | 0.44     | 2.75        | 7      | 1     |
| 1:B:102:ASN:HD22 | 1:B:105:ALA:C    | 0.44     | 2.20        | 7      | 1     |
| 1:A:102:ASN:ND2  | 1:A:105:ALA:O    | 0.44     | 2.45        | 8      | 3     |
| 1:B:147:GLY:O    | 1:B:149:ASP:N    | 0.44     | 2.51        | 10     | 1     |
| 1:B:95:TRP:CE2   | 1:B:97:VAL:HG22  | 0.44     | 2.47        | 8      | 1     |
| 1:A:114:LYS:HB3  | 1:A:117:VAL:HB   | 0.44     | 1.89        | 6      | 4     |
| 1:A:143:THR:O    | 1:A:145:PRO:HD3  | 0.44     | 2.12        | 6      | 2     |
| 1:B:99:LEU:HD23  | 1:B:140:ARG:NH1  | 0.44     | 2.28        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:149:ASP:OD1  | 1:B:151:THR:N    | 0.44     | 2.48        | 9      | 1     |
| 1:A:109:LEU:HG   | 1:A:110:THR:N    | 0.43     | 2.27        | 2      | 1     |
| 1:A:140:ARG:NH2  | 1:A:141:LYS:O    | 0.43     | 2.46        | 8      | 1     |
| 1:A:140:ARG:CZ   | 1:A:140:ARG:HB3  | 0.43     | 2.43        | 2      | 1     |
| 1:A:102:ASN:ND2  | 1:A:102:ASN:C    | 0.43     | 2.73        | 6      | 1     |
| 1:B:149:ASP:OD1  | 1:B:149:ASP:N    | 0.43     | 2.49        | 1      | 2     |
| 1:A:95:TRP:CZ2   | 1:A:165:VAL:HG23 | 0.43     | 2.49        | 2      | 1     |
| 1:A:102:ASN:OD1  | 1:A:161:GLY:CA   | 0.43     | 2.67        | 8      | 2     |
| 1:B:95:TRP:CG    | 1:B:169:MET:HE3  | 0.43     | 2.48        | 8      | 1     |
| 1:B:104:PHE:CE2  | 1:B:136:ARG:NH2  | 0.43     | 2.86        | 8      | 1     |
| 1:A:102:ASN:O    | 1:A:103:HIS:C    | 0.43     | 2.62        | 8      | 3     |
| 1:A:140:ARG:NH2  | 1:B:131:HIS:ND1  | 0.43     | 2.66        | 4      | 1     |
| 1:B:147:GLY:O    | 1:B:169:MET:HE2  | 0.43     | 2.13        | 6      | 1     |
| 1:B:104:PHE:CD2  | 1:B:136:ARG:NH2  | 0.43     | 2.86        | 8      | 1     |
| 1:A:96:ARG:CZ    | 1:A:96:ARG:HB3   | 0.43     | 2.44        | 9      | 1     |
| 1:A:100:ASP:O    | 1:A:100:ASP:CG   | 0.43     | 2.61        | 9      | 1     |
| 1:A:102:ASN:HB3  | 1:A:109:LEU:CD1  | 0.43     | 2.43        | 10     | 1     |
| 1:A:107:ASP:C    | 1:A:109:LEU:H    | 0.43     | 2.21        | 1      | 2     |
| 1:A:124:HIS:O    | 1:A:135:SER:OG   | 0.43     | 2.35        | 2      | 1     |
| 1:A:102:ASN:ND2  | 1:A:102:ASN:O    | 0.43     | 2.51        | 8      | 1     |
| 1:A:140:ARG:NH2  | 1:A:141:LYS:N    | 0.43     | 2.66        | 8      | 1     |
| 1:A:140:ARG:CZ   | 1:A:142:TYR:CE1  | 0.43     | 3.01        | 8      | 1     |
| 1:B:140:ARG:CZ   | 1:B:140:ARG:CB   | 0.43     | 2.97        | 8      | 1     |
| 1:A:100:ASP:O    | 1:A:101:VAL:HG22 | 0.43     | 2.14        | 9      | 1     |
| 1:B:102:ASN:OD1  | 1:B:157:LEU:HD13 | 0.43     | 2.13        | 9      | 2     |
| 1:B:103:HIS:ND1  | 1:B:103:HIS:N    | 0.43     | 2.67        | 4      | 1     |
| 1:B:134:ILE:HD11 | 1:B:136:ARG:NH1  | 0.43     | 2.29        | 9      | 1     |
| 1:A:141:LYS:NZ   | 1:A:141:LYS:HB2  | 0.43     | 2.28        | 1      | 2     |
| 1:B:160:GLU:CD   | 1:B:160:GLU:N    | 0.43     | 2.77        | 1      | 1     |
| 1:A:94:ARG:HH21  | 1:A:166:GLU:CD   | 0.43     | 2.22        | 4      | 1     |
| 1:B:104:PHE:HB3  | 1:B:136:ARG:CZ   | 0.43     | 2.44        | 10     | 1     |
| 1:A:134:ILE:HA   | 1:B:139:THR:O    | 0.42     | 2.13        | 4      | 1     |
| 1:B:167:ALA:C    | 1:B:169:MET:H    | 0.42     | 2.22        | 2      | 1     |
| 1:A:94:ARG:NH2   | 1:A:166:GLU:OE2  | 0.42     | 2.44        | 2      | 1     |
| 1:B:102:ASN:O    | 1:B:103:HIS:C    | 0.42     | 2.62        | 4      | 3     |
| 1:B:117:VAL:HG13 | 1:B:143:THR:HG23 | 0.42     | 1.89        | 5      | 1     |
| 1:B:100:ASP:O    | 1:B:100:ASP:CG   | 0.42     | 2.62        | 10     | 1     |
| 1:B:119:GLU:HG2  | 1:B:141:LYS:CB   | 0.42     | 2.45        | 4      | 1     |
| 1:A:95:TRP:O     | 1:A:166:GLU:HA   | 0.42     | 2.13        | 7      | 1     |
| 1:B:136:ARG:O    | 1:B:136:ARG:NE   | 0.42     | 2.48        | 10     | 1     |
| 1:A:149:ASP:OD2  | 1:A:152:GLN:N    | 0.42     | 2.45        | 1      | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:158:SER:C    | 1:A:160:GLU:H   | 0.42     | 2.22        | 2      | 1     |
| 1:A:127:ARG:O    | 1:A:134:ILE:N   | 0.42     | 2.47        | 9      | 1     |
| 1:A:133:TYR:O    | 1:B:141:LYS:N   | 0.42     | 2.46        | 10     | 1     |
| 1:A:104:PHE:CE2  | 1:A:136:ARG:NH2 | 0.42     | 2.88        | 1      | 1     |
| 1:A:119:GLU:OE2  | 1:A:141:LYS:NZ  | 0.42     | 2.39        | 6      | 1     |
| 1:B:129:ASP:CG   | 1:B:130:GLU:H   | 0.42     | 2.23        | 6      | 1     |
| 1:A:169:MET:CB   | 1:A:170:PRO:HD2 | 0.42     | 2.45        | 8      | 1     |
| 1:B:95:TRP:N     | 1:B:167:ALA:O   | 0.42     | 2.52        | 2      | 1     |
| 1:B:157:LEU:HD12 | 1:B:158:SER:H   | 0.42     | 1.75        | 8      | 1     |
| 1:B:142:TYR:N    | 1:B:142:TYR:CD1 | 0.42     | 2.88        | 3      | 1     |
| 1:A:124:HIS:HB3  | 1:A:127:ARG:NH2 | 0.42     | 2.30        | 7      | 1     |
| 1:B:104:PHE:HB3  | 1:B:136:ARG:NH1 | 0.42     | 2.30        | 10     | 1     |
| 1:B:127:ARG:NH1  | 1:B:127:ARG:CB  | 0.41     | 2.82        | 7      | 1     |
| 1:A:140:ARG:NE   | 1:A:142:TYR:CZ  | 0.41     | 2.88        | 8      | 1     |
| 1:B:95:TRP:CB    | 1:B:169:MET:HG2 | 0.41     | 2.45        | 8      | 1     |
| 1:A:124:HIS:CD2  | 1:A:127:ARG:HG3 | 0.41     | 2.50        | 10     | 1     |
| 1:A:102:ASN:C    | 1:A:104:PHE:N   | 0.41     | 2.78        | 9      | 2     |
| 1:A:101:VAL:N    | 1:A:103:HIS:CE1 | 0.41     | 2.88        | 3      | 1     |
| 1:B:158:SER:HB2  | 1:B:162:THR:CG2 | 0.41     | 2.45        | 8      | 1     |
| 1:B:108:GLU:HB3  | 1:B:123:LYS:O   | 0.41     | 2.15        | 10     | 1     |
| 1:A:99:LEU:HD23  | 1:A:140:ARG:HD3 | 0.41     | 1.93        | 4      | 1     |
| 1:B:117:VAL:CG1  | 1:B:141:LYS:HG3 | 0.41     | 2.46        | 7      | 1     |
| 1:A:140:ARG:NH1  | 1:B:134:ILE:HB  | 0.41     | 2.30        | 10     | 2     |
| 1:B:95:TRP:O     | 1:B:166:GLU:HA  | 0.41     | 2.16        | 2      | 1     |
| 1:A:119:GLU:HG2  | 1:A:141:LYS:CB  | 0.41     | 2.45        | 3      | 2     |
| 1:A:104:PHE:CZ   | 1:A:136:ARG:NH1 | 0.41     | 2.89        | 6      | 1     |
| 1:A:99:LEU:CD2   | 1:A:140:ARG:CB  | 0.41     | 2.98        | 8      | 1     |
| 1:A:124:HIS:CD2  | 1:A:127:ARG:CG  | 0.41     | 3.03        | 1      | 1     |
| 1:A:102:ASN:HB3  | 1:A:161:GLY:O   | 0.41     | 2.15        | 6      | 1     |
| 1:A:132:GLY:HA3  | 1:B:142:TYR:CZ  | 0.41     | 2.50        | 5      | 1     |
| 1:A:160:GLU:O    | 1:A:162:THR:N   | 0.41     | 2.54        | 7      | 1     |
| 1:A:134:ILE:HD12 | 1:B:140:ARG:CZ  | 0.41     | 2.45        | 2      | 1     |
| 1:B:104:PHE:CE1  | 1:B:127:ARG:NH1 | 0.41     | 2.89        | 2      | 2     |
| 1:A:103:HIS:CD2  | 1:A:103:HIS:C   | 0.41     | 2.99        | 6      | 1     |
| 1:B:110:THR:N    | 1:B:121:THR:O   | 0.41     | 2.53        | 7      | 1     |
| 1:B:160:GLU:CD   | 1:B:160:GLU:H   | 0.41     | 2.24        | 9      | 1     |
| 1:A:124:HIS:CG   | 1:A:127:ARG:HD3 | 0.41     | 2.51        | 10     | 1     |
| 1:B:102:ASN:HD21 | 1:B:106:PRO:HA  | 0.41     | 1.75        | 10     | 1     |
| 1:B:157:LEU:HD12 | 1:B:162:THR:O   | 0.41     | 2.16        | 3      | 1     |
| 1:B:157:LEU:HD11 | 1:B:161:GLY:HA2 | 0.41     | 1.91        | 3      | 1     |
| 1:B:114:LYS:O    | 1:B:117:VAL:CB  | 0.41     | 2.68        | 7      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:B:127:ARG:NH1 | 1:B:134:ILE:HG23 | 0.40     | 2.31        | 7      | 1     |
| 1:A:119:GLU:HG2 | 1:A:141:LYS:HA   | 0.40     | 1.92        | 8      | 1     |
| 1:B:145:PRO:CD  | 1:B:146:PRO:HD2  | 0.40     | 2.46        | 5      | 1     |
| 1:A:141:LYS:HZ3 | 1:A:141:LYS:HB2  | 0.40     | 1.75        | 6      | 1     |
| 1:B:100:ASP:OD2 | 1:B:103:HIS:NE2  | 0.40     | 2.45        | 7      | 1     |
| 1:A:119:GLU:HG2 | 1:A:141:LYS:HB2  | 0.40     | 1.94        | 8      | 1     |
| 1:B:124:HIS:CD2 | 1:B:124:HIS:N    | 0.40     | 2.82        | 8      | 1     |
| 1:B:100:ASP:C   | 1:B:103:HIS:CE1  | 0.40     | 2.99        | 9      | 1     |
| 1:B:124:HIS:O   | 1:B:135:SER:OG   | 0.40     | 2.35        | 4      | 1     |
| 1:A:95:TRP:CD1  | 1:A:95:TRP:O     | 0.40     | 2.74        | 6      | 1     |
| 1:A:102:ASN:C   | 1:A:102:ASN:HD22 | 0.40     | 2.22        | 9      | 1     |
| 1:A:149:ASP:OD1 | 1:A:152:GLN:N    | 0.40     | 2.49        | 9      | 1     |
| 1:B:136:ARG:HD2 | 1:B:138:PHE:CE2  | 0.40     | 2.51        | 5      | 1     |
| 1:B:112:LYS:NZ  | 1:B:119:GLU:CD   | 0.40     | 2.79        | 4      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured     | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|------------|-------------|----|
| 1   | A     | 73/98 (74%)     | 58±2 (80±3%) | 10±2 (13±3%) | 5±1 (7±2%) | 2           | 16 |
| 1   | B     | 76/98 (78%)     | 61±2 (81±3%) | 9±2 (12±3%)  | 6±1 (8±2%) | 1           | 15 |
| All | All   | 1490/1960 (76%) | 1197 (80%)   | 185 (12%)    | 108 (7%)   | 2           | 15 |

All 27 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     | 126 | GLU  | 10             |
| 1   | B     | 146 | PRO  | 10             |
| 1   | A     | 101 | VAL  | 9              |
| 1   | B     | 101 | VAL  | 9              |
| 1   | B     | 126 | GLU  | 8              |
| 1   | A     | 102 | ASN  | 7              |
| 1   | A     | 146 | PRO  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 102 | ASN  | 5              |
| 1   | B     | 160 | GLU  | 5              |
| 1   | A     | 147 | GLY  | 4              |
| 1   | A     | 160 | GLU  | 4              |
| 1   | A     | 94  | ARG  | 3              |
| 1   | B     | 106 | PRO  | 3              |
| 1   | B     | 115 | ASP  | 3              |
| 1   | B     | 94  | ARG  | 3              |
| 1   | B     | 147 | GLY  | 3              |
| 1   | A     | 170 | PRO  | 2              |
| 1   | B     | 169 | MET  | 2              |
| 1   | B     | 100 | ASP  | 2              |
| 1   | B     | 148 | VAL  | 2              |
| 1   | A     | 167 | ALA  | 1              |
| 1   | B     | 103 | HIS  | 1              |
| 1   | A     | 150 | PRO  | 1              |
| 1   | B     | 161 | GLY  | 1              |
| 1   | A     | 106 | PRO  | 1              |
| 1   | A     | 161 | GLY  | 1              |
| 1   | A     | 115 | ASP  | 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     | 66/88 (75%)     | 38±3 (58±4%) | 28±3 (42±4%) | 0           | 4 |
| 1   | B     | 69/88 (78%)     | 38±3 (56±4%) | 30±3 (44±4%) | 0           | 3 |
| All | All   | 1350/1760 (77%) | 765 (57%)    | 585 (43%)    | 0           | 3 |

All 98 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     | 97  | VAL  | 10             |
| 1   | A     | 99  | LEU  | 10             |
| 1   | A     | 102 | ASN  | 10             |
| 1   | A     | 109 | LEU  | 10             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 121 | THR  | 10             |
| 1   | A     | 123 | LYS  | 10             |
| 1   | A     | 134 | ILE  | 10             |
| 1   | A     | 139 | THR  | 10             |
| 1   | A     | 143 | THR  | 10             |
| 1   | A     | 148 | VAL  | 10             |
| 1   | A     | 151 | THR  | 10             |
| 1   | A     | 154 | SER  | 10             |
| 1   | A     | 156 | SER  | 10             |
| 1   | B     | 97  | VAL  | 10             |
| 1   | B     | 99  | LEU  | 10             |
| 1   | B     | 109 | LEU  | 10             |
| 1   | B     | 110 | THR  | 10             |
| 1   | B     | 121 | THR  | 10             |
| 1   | B     | 134 | ILE  | 10             |
| 1   | B     | 135 | SER  | 10             |
| 1   | B     | 139 | THR  | 10             |
| 1   | B     | 140 | ARG  | 10             |
| 1   | B     | 148 | VAL  | 10             |
| 1   | B     | 151 | THR  | 10             |
| 1   | B     | 154 | SER  | 10             |
| 1   | B     | 155 | SER  | 10             |
| 1   | B     | 156 | SER  | 10             |
| 1   | B     | 164 | THR  | 10             |
| 1   | A     | 101 | VAL  | 9              |
| 1   | A     | 136 | ARG  | 9              |
| 1   | B     | 102 | ASN  | 9              |
| 1   | B     | 114 | LYS  | 9              |
| 1   | B     | 123 | LYS  | 9              |
| 1   | B     | 143 | THR  | 9              |
| 1   | A     | 155 | SER  | 9              |
| 1   | A     | 110 | THR  | 8              |
| 1   | A     | 169 | MET  | 8              |
| 1   | A     | 158 | SER  | 8              |
| 1   | B     | 158 | SER  | 8              |
| 1   | A     | 95  | TRP  | 7              |
| 1   | A     | 114 | LYS  | 7              |
| 1   | A     | 140 | ARG  | 7              |
| 1   | B     | 101 | VAL  | 7              |
| 1   | B     | 111 | VAL  | 7              |
| 1   | B     | 113 | THR  | 7              |
| 1   | B     | 169 | MET  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 95  | TRP  | 7              |
| 1   | A     | 112 | LYS  | 6              |
| 1   | A     | 164 | THR  | 6              |
| 1   | B     | 166 | GLU  | 6              |
| 1   | A     | 125 | GLU  | 6              |
| 1   | A     | 120 | ILE  | 5              |
| 1   | B     | 126 | GLU  | 5              |
| 1   | B     | 129 | ASP  | 5              |
| 1   | B     | 130 | GLU  | 5              |
| 1   | A     | 113 | THR  | 5              |
| 1   | A     | 103 | HIS  | 4              |
| 1   | A     | 127 | ARG  | 4              |
| 1   | A     | 135 | SER  | 4              |
| 1   | B     | 124 | HIS  | 4              |
| 1   | B     | 125 | GLU  | 4              |
| 1   | B     | 127 | ARG  | 4              |
| 1   | A     | 166 | GLU  | 4              |
| 1   | B     | 112 | LYS  | 4              |
| 1   | B     | 136 | ARG  | 4              |
| 1   | A     | 111 | VAL  | 4              |
| 1   | A     | 141 | LYS  | 3              |
| 1   | B     | 94  | ARG  | 3              |
| 1   | B     | 103 | HIS  | 3              |
| 1   | B     | 107 | ASP  | 3              |
| 1   | B     | 108 | GLU  | 3              |
| 1   | B     | 138 | PHE  | 3              |
| 1   | A     | 115 | ASP  | 3              |
| 1   | A     | 165 | VAL  | 3              |
| 1   | B     | 120 | ILE  | 3              |
| 1   | B     | 141 | LYS  | 3              |
| 1   | B     | 152 | GLN  | 3              |
| 1   | B     | 100 | ASP  | 3              |
| 1   | A     | 98  | SER  | 3              |
| 1   | A     | 119 | GLU  | 2              |
| 1   | B     | 117 | VAL  | 2              |
| 1   | A     | 104 | PHE  | 2              |
| 1   | A     | 96  | ARG  | 2              |
| 1   | A     | 100 | ASP  | 2              |
| 1   | A     | 126 | GLU  | 2              |
| 1   | A     | 117 | VAL  | 2              |
| 1   | B     | 119 | GLU  | 1              |
| 1   | B     | 149 | ASP  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 162 | THR  | 1              |
| 1   | A     | 163 | LEU  | 1              |
| 1   | B     | 104 | PHE  | 1              |
| 1   | B     | 115 | ASP  | 1              |
| 1   | A     | 149 | ASP  | 1              |
| 1   | A     | 152 | GLN  | 1              |
| 1   | B     | 142 | TYR  | 1              |
| 1   | A     | 94  | ARG  | 1              |
| 1   | A     | 124 | HIS  | 1              |
| 1   | B     | 128 | GLN  | 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 20% for the well-defined parts and 19% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

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

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 490 |
| Number of shifts mapped to atoms        | 490 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 90       | $0.41 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 84       | $0.84 \pm 0.21$                 | Should be applied          |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 77       | $-0.47 \pm 0.34$                | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 20%, i.e. 409 atoms were assigned a chemical shift out of a possible 1997. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 219/729 (30%)  | 83/295 (28%)  | 72/298 (24%)    | 64/136 (47%)    |
| Sidechain | 188/1133 (17%) | 118/734 (16%) | 68/356 (19%)    | 2/43 (5%)       |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 2/135 (1%)     | 1/68 (1%)      | 0/60 (0%)       | 1/7 (14%)       |
| Overall  | 409/1997 (20%) | 202/1097 (18%) | 140/714 (20%)   | 67/186 (36%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 490 atoms were assigned a chemical shift out of a possible 2598. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 269/964 (28%)  | 102/390 (26%)  | 90/392 (23%)    | 77/182 (42%)    |
| Sidechain | 219/1478 (15%) | 130/958 (14%)  | 86/464 (19%)    | 3/56 (5%)       |
| Aromatic  | 2/156 (1%)     | 1/80 (1%)      | 0/66 (0%)       | 1/10 (10%)      |
| Overall   | 490/2598 (19%) | 233/1428 (16%) | 176/922 (19%)   | 81/248 (33%)    |

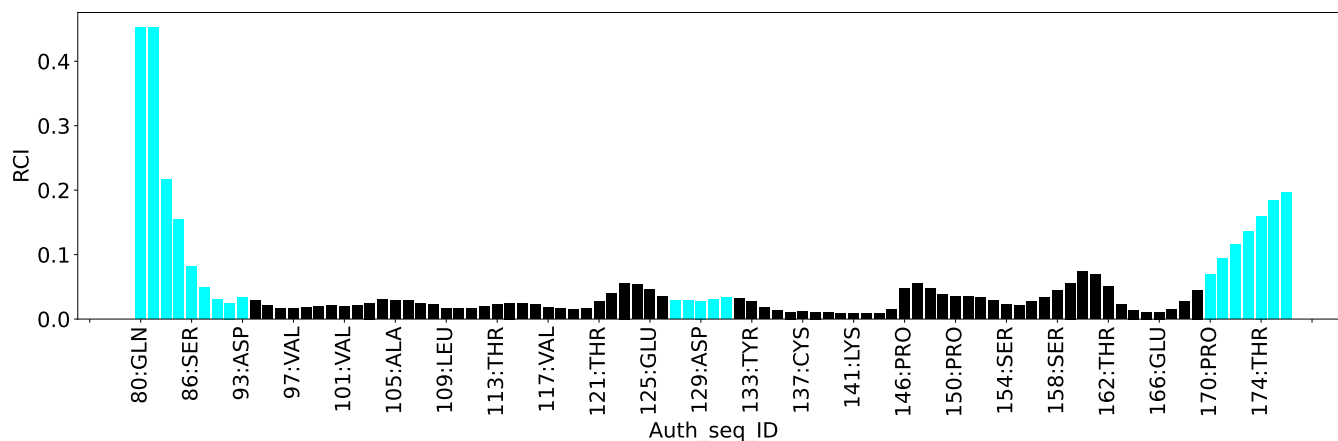
#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 4298  |
| Intra-residue ( $ i-j =0$ )                              | 899   |
| Sequential ( $ i-j =1$ )                                 | 1094  |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 533   |
| Long range ( $ i-j \geq 5$ )                             | 1507  |
| Inter-chain                                              | 264   |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 1     |
| Total dihedral-angle restraints                          | 230   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 23.1  |
| Number of long range restraints per residue <sup>1</sup> | 7.7   |

<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)  | 177.0                                  | 0.2     |
| 0.2-0.5 (Medium) | 233.9                                  | 0.5     |
| >0.5 (Large)     | 169.1                                  | 7.17    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 12.8                                   | 9.77    |
| 10.0-20.0 (Medium) | 0.1                                    | 10.01   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

### 9.1 Summary of distance violations ⓘ

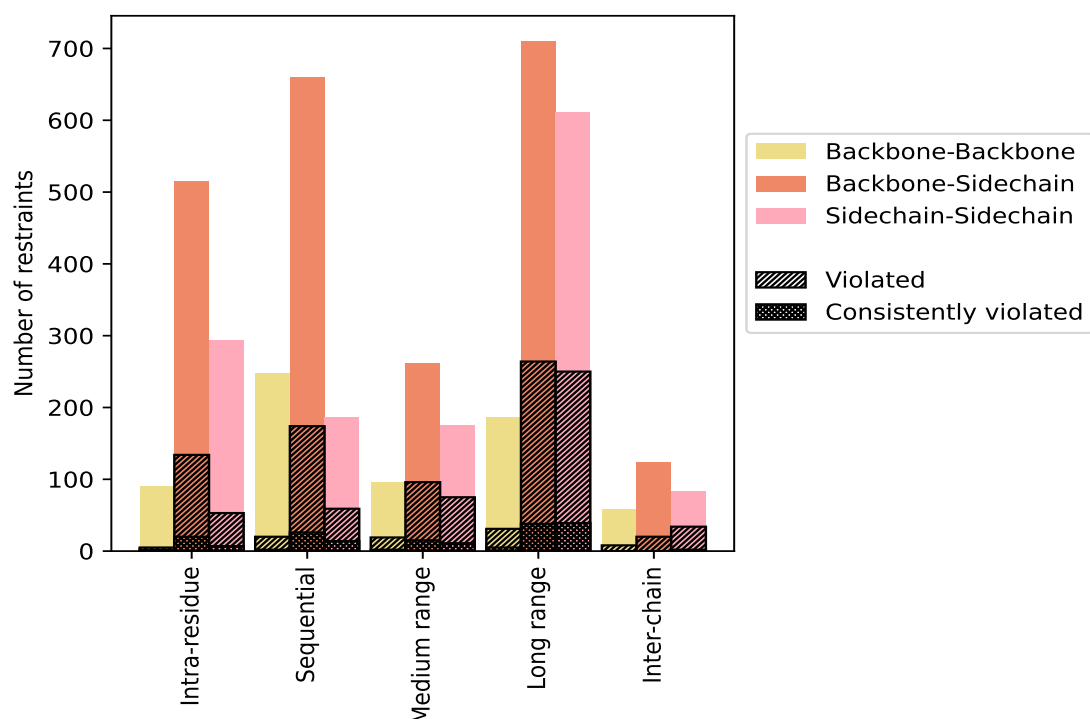
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type                         | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|----------------------------------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                        |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| Intra-residue ( $ i-j =0$ )            | 899   | 20.9           | 192                   | 21.4           | 4.5            | 29                                 | 3.2            | 0.7            |
| Backbone-Backbone                      | 90    | 2.1            | 5                     | 5.6            | 0.1            | 2                                  | 2.2            | 0.0            |
| Backbone-Sidechain                     | 515   | 12.0           | 134                   | 26.0           | 3.1            | 20                                 | 3.9            | 0.5            |
| Sidechain-Sidechain                    | 294   | 6.8            | 53                    | 18.0           | 1.2            | 7                                  | 2.4            | 0.2            |
| Sequential ( $ i-j =1$ )               | 1094  | 25.5           | 253                   | 23.1           | 5.9            | 42                                 | 3.8            | 1.0            |
| Backbone-Backbone                      | 248   | 5.8            | 20                    | 8.1            | 0.5            | 2                                  | 0.8            | 0.0            |
| Backbone-Sidechain                     | 660   | 15.4           | 174                   | 26.4           | 4.0            | 26                                 | 3.9            | 0.6            |
| Sidechain-Sidechain                    | 186   | 4.3            | 59                    | 31.7           | 1.4            | 14                                 | 7.5            | 0.3            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 533   | 12.4           | 190                   | 35.6           | 4.4            | 28                                 | 5.3            | 0.7            |
| Backbone-Backbone                      | 96    | 2.2            | 19                    | 19.8           | 0.4            | 2                                  | 2.1            | 0.0            |
| Backbone-Sidechain                     | 262   | 6.1            | 96                    | 36.6           | 2.2            | 15                                 | 5.7            | 0.3            |
| Sidechain-Sidechain                    | 175   | 4.1            | 75                    | 42.9           | 1.7            | 11                                 | 6.3            | 0.3            |
| Long range ( $ i-j \geq 5$ )           | 1507  | 35.1           | 545                   | 36.2           | 12.7           | 82                                 | 5.4            | 1.9            |
| Backbone-Backbone                      | 186   | 4.3            | 31                    | 16.7           | 0.7            | 5                                  | 2.7            | 0.1            |
| Backbone-Sidechain                     | 710   | 16.5           | 264                   | 37.2           | 6.1            | 38                                 | 5.4            | 0.9            |
| Sidechain-Sidechain                    | 611   | 14.2           | 250                   | 40.9           | 5.8            | 39                                 | 6.4            | 0.9            |
| Inter-chain                            | 264   | 6.1            | 62                    | 23.5           | 1.4            | 2                                  | 0.8            | 0.0            |
| Backbone-Backbone                      | 58    | 1.3            | 8                     | 13.8           | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 124   | 2.9            | 20                    | 16.1           | 0.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 82    | 1.9            | 34                    | 41.5           | 0.8            | 2                                  | 2.4            | 0.0            |
| Hydrogen bond                          | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Disulfide bond                         | 1     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 4298  | 100.0          | 1242                  | 28.9           | 28.9           | 183                                | 4.3            | 4.3            |
| Backbone-Backbone                      | 678   | 15.8           | 83                    | 12.2           | 1.9            | 11                                 | 1.6            | 0.3            |
| Backbone-Sidechain                     | 2271  | 52.8           | 688                   | 30.3           | 16.0           | 99                                 | 4.4            | 2.3            |
| Sidechain-Sidechain                    | 1349  | 31.4           | 471                   | 34.9           | 11.0           | 73                                 | 5.4            | 1.7            |

<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

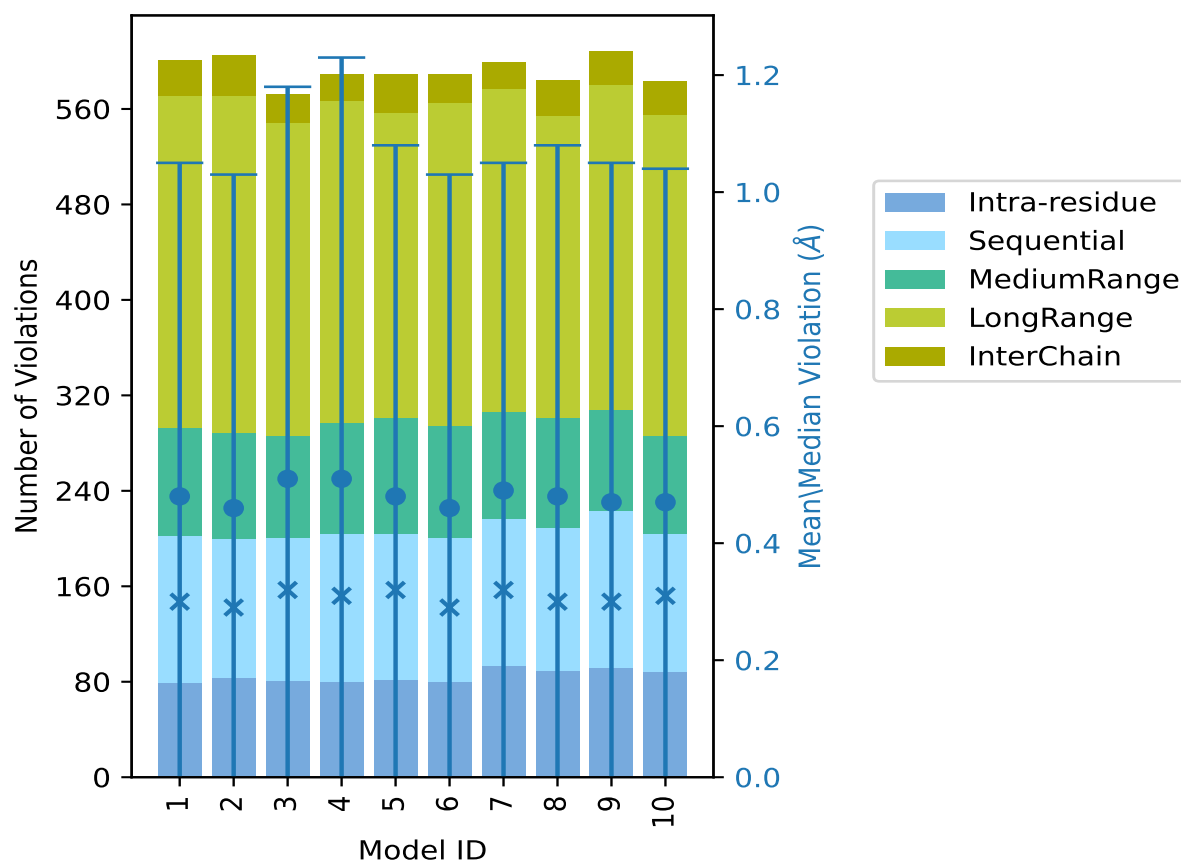
## 9.2 Distance violation statistics for each model [i](#)

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        | 79                   | 123             | 91              | 278             | 30              | 601   | 0.48     | 5.27    | 0.57                | 0.3        |
| 2        | 83                   | 117             | 89              | 282             | 34              | 605   | 0.46     | 5.46    | 0.57                | 0.29       |
| 3        | 81                   | 120             | 85              | 262             | 24              | 572   | 0.51     | 6.11    | 0.67                | 0.32       |
| 4        | 80                   | 124             | 93              | 270             | 22              | 589   | 0.51     | 7.16    | 0.72                | 0.31       |
| 5        | 82                   | 122             | 97              | 256             | 32              | 589   | 0.48     | 7.17    | 0.6                 | 0.32       |
| 6        | 80                   | 121             | 94              | 270             | 24              | 589   | 0.46     | 6.06    | 0.57                | 0.29       |
| 7        | 93                   | 124             | 89              | 271             | 22              | 599   | 0.49     | 6.94    | 0.56                | 0.32       |
| 8        | 89                   | 120             | 92              | 253             | 30              | 584   | 0.48     | 6.54    | 0.6                 | 0.3        |
| 9        | 92                   | 131             | 85              | 272             | 28              | 608   | 0.47     | 6.42    | 0.58                | 0.3        |
| 10       | 88                   | 116             | 82              | 269             | 28              | 583   | 0.47     | 5.28    | 0.57                | 0.31       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3055(IR:707, SQ:841, MR:343, LR:962, IC:202) 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>       | %    |
| 41                            | 67              | 42              | 110             | 14              | 274   | 1                        | 10.0 |
| 31                            | 32              | 26              | 62              | 6               | 157   | 2                        | 20.0 |
| 30                            | 22              | 18              | 70              | 10              | 150   | 3                        | 30.0 |

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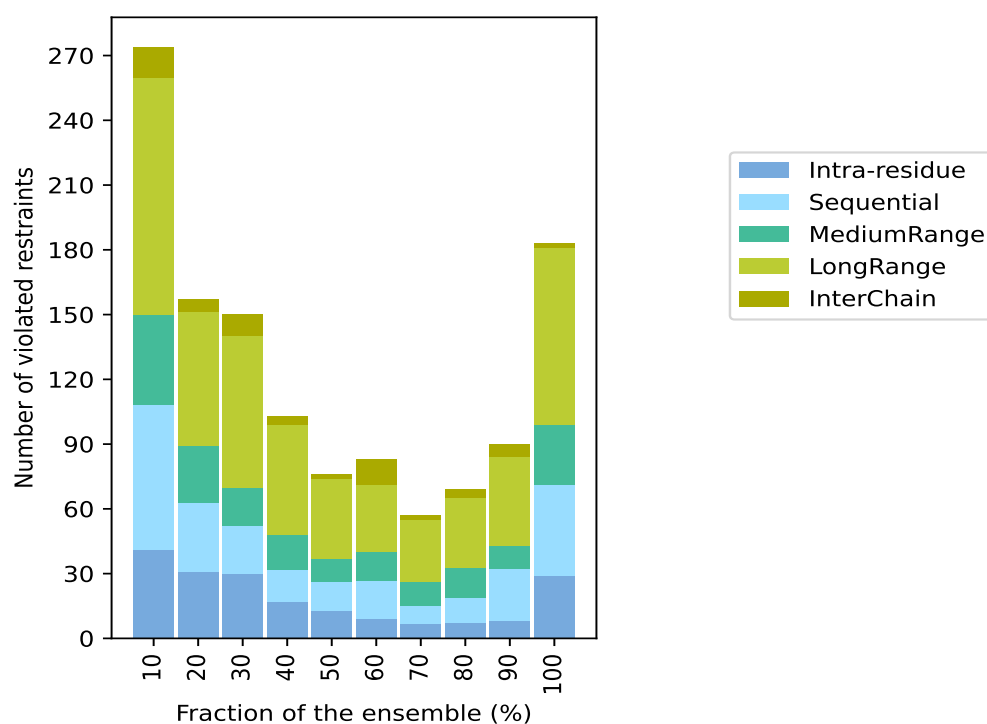
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 17                            | 15              | 16              | 51              | 4               | 103   | 4                        | 40.0  |
| 13                            | 13              | 11              | 37              | 2               | 76    | 5                        | 50.0  |
| 9                             | 18              | 13              | 31              | 12              | 83    | 6                        | 60.0  |
| 7                             | 8               | 11              | 29              | 2               | 57    | 7                        | 70.0  |
| 7                             | 12              | 14              | 32              | 4               | 69    | 8                        | 80.0  |
| 8                             | 24              | 11              | 41              | 6               | 90    | 9                        | 90.0  |
| 29                            | 42              | 28              | 82              | 2               | 183   | 10                       | 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](#)

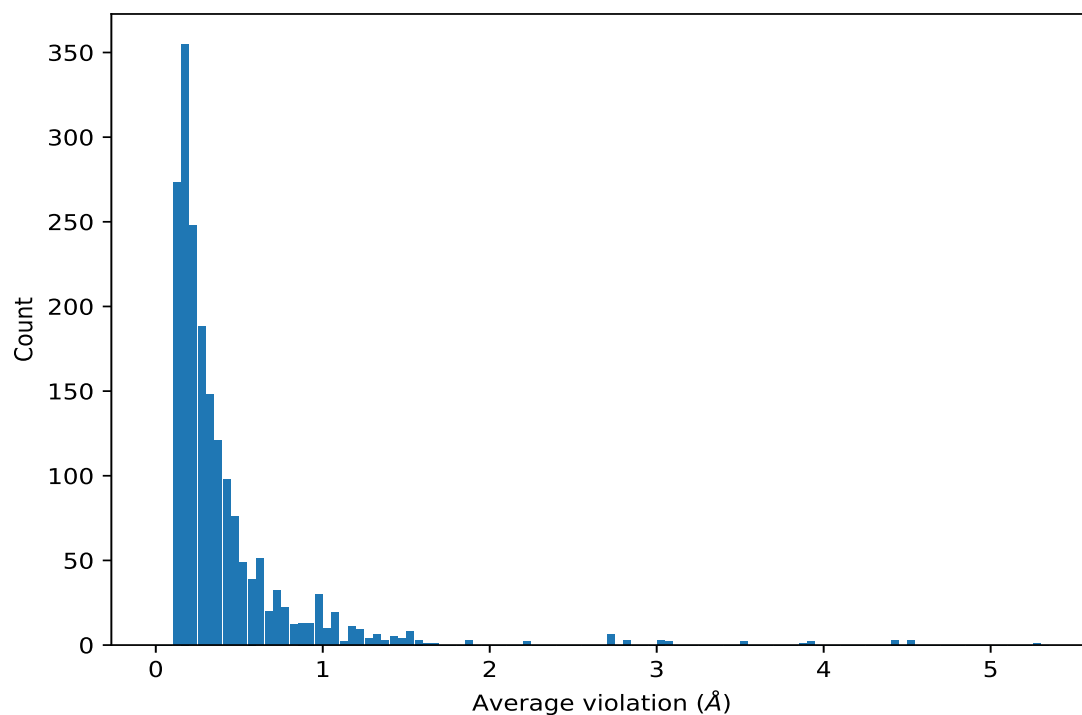


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA   | 10                  | 5.28     | 1.15                | 5.49       |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG2  | 10                  | 3.9      | 1.89                | 4.2        |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG3  | 10                  | 3.9      | 1.89                | 4.2        |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA   | 10                  | 3.88     | 1.42                | 3.52       |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1   | 10                  | 3.04     | 1.51                | 3.45       |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2   | 10                  | 3.04     | 1.51                | 3.45       |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3   | 10                  | 3.04     | 1.51                | 3.45       |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG2  | 10                  | 2.74     | 1.96                | 3.14       |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG3  | 10                  | 2.74     | 1.96                | 3.14       |
| (1,17)   | 1:93:A:ASP:HA   | 1:169:A:MET:HG2  | 10                  | 1.61     | 0.97                | 1.39       |
| (1,4)    | 1:89:A:ARG:HB3  | 1:90:A:HIS:HB3   | 10                  | 1.57     | 0.47                | 1.66       |
| (1,4)    | 1:89:A:ARG:HB2  | 1:90:A:HIS:HB3   | 10                  | 1.57     | 0.47                | 1.66       |
| (1,286)  | 1:105:A:ALA:HA  | 1:108:A:GLU:HB2  | 10                  | 1.55     | 0.06                | 1.56       |
| (1,110)  | 1:96:A:ARG:HG3  | 1:166:A:GLU:HB3  | 10                  | 1.54     | 0.16                | 1.5        |
| (1,328)  | 1:106:A:PRO:HD2 | 1:157:A:LEU:HD23 | 10                  | 1.54     | 0.14                | 1.49       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD22 | 10                  | 1.54     | 0.14                | 1.49       |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD21 | 10                  | 1.54     | 0.14                | 1.49       |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 10                  | 1.51     | 0.21                | 1.52       |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD21 | 10                  | 1.48     | 0.08                | 1.5        |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD22 | 10                  | 1.48     | 0.08                | 1.5        |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD23 | 10                  | 1.48     | 0.08                | 1.5        |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 10                  | 1.37     | 0.37                | 1.46       |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD12 | 10                  | 1.37     | 0.31                | 1.37       |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD11 | 10                  | 1.37     | 0.31                | 1.37       |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD13 | 10                  | 1.3      | 0.4                 | 1.44       |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD12 | 10                  | 1.3      | 0.4                 | 1.44       |
| (1,2608) | 1:106:B:PRO:HG2  | 1:157:B:LEU:HD11 | 10                  | 1.3      | 0.4                 | 1.44       |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD11 | 10                  | 1.3      | 0.4                 | 1.44       |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 10                  | 1.29     | 0.27                | 1.28       |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 10                  | 1.26     | 0.46                | 1.31       |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 10                  | 1.24     | 0.29                | 1.34       |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 10                  | 1.24     | 0.29                | 1.34       |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 10                  | 1.17     | 0.19                | 1.18       |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 10                  | 1.17     | 0.19                | 1.18       |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 10                  | 1.17     | 0.19                | 1.18       |
| (1,2538) | 1:99:B:LEU:HD11  | 1:112:B:LYS:HG3  | 10                  | 1.17     | 0.19                | 1.18       |
| (1,2538) | 1:99:B:LEU:HD12  | 1:112:B:LYS:HG3  | 10                  | 1.17     | 0.19                | 1.18       |
| (1,2538) | 1:99:B:LEU:HD13  | 1:112:B:LYS:HG3  | 10                  | 1.17     | 0.19                | 1.18       |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 10                  | 1.17     | 0.06                | 1.15       |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 10                  | 1.17     | 0.06                | 1.15       |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 10                  | 1.17     | 0.06                | 1.15       |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 10                  | 1.12     | 0.22                | 1.19       |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 10                  | 1.12     | 0.22                | 1.19       |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 10                  | 1.09     | 0.09                | 1.08       |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 10                  | 1.09     | 0.09                | 1.08       |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 10                  | 1.09     | 0.09                | 1.08       |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 10                  | 1.06     | 0.25                | 1.11       |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 10                  | 1.05     | 0.26                | 1.1        |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 10                  | 1.05     | 0.26                | 1.1        |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 10                  | 1.05     | 0.26                | 1.1        |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 10                  | 1.05     | 0.48                | 1.27       |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 10                  | 1.05     | 0.44                | 1.22       |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 10                  | 1.04     | 0.19                | 1.04       |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 10                  | 1.04     | 0.19                | 1.04       |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 10                  | 1.04     | 0.19                | 1.04       |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 10                  | 1.01     | 0.24                | 1.17       |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 10                  | 0.99     | 0.08                | 0.98       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 10                  | 0.99     | 0.08                | 0.98       |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 10                  | 0.99     | 0.08                | 0.98       |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 10                  | 0.98     | 0.34                | 0.86       |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 10                  | 0.98     | 0.34                | 0.86       |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 10                  | 0.98     | 0.34                | 0.86       |
| (1,257)  | 1:99:A:LEU:HD11  | 1:112:A:LYS:HG3  | 10                  | 0.98     | 0.34                | 0.86       |
| (1,257)  | 1:99:A:LEU:HD12  | 1:112:A:LYS:HG3  | 10                  | 0.98     | 0.34                | 0.86       |
| (1,257)  | 1:99:A:LEU:HD13  | 1:112:A:LYS:HG3  | 10                  | 0.98     | 0.34                | 0.86       |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 10                  | 0.97     | 0.06                | 0.96       |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 10                  | 0.97     | 0.06                | 0.96       |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 10                  | 0.97     | 0.06                | 0.96       |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 10                  | 0.96     | 0.28                | 1.04       |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 10                  | 0.93     | 0.15                | 0.92       |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 10                  | 0.93     | 0.32                | 1.0        |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 10                  | 0.91     | 0.19                | 0.98       |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 10                  | 0.89     | 0.48                | 0.82       |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG3  | 10                  | 0.89     | 0.48                | 0.82       |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 10                  | 0.87     | 0.18                | 0.9        |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 10                  | 0.87     | 0.18                | 0.9        |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 10                  | 0.87     | 0.18                | 0.9        |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 10                  | 0.87     | 0.23                | 0.94       |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 10                  | 0.87     | 0.19                | 0.88       |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 10                  | 0.86     | 0.17                | 0.86       |
| (1,474)  | 1:112:A:LYS:HE3  | 1:114:A:LYS:HB3  | 10                  | 0.84     | 0.14                | 0.86       |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 10                  | 0.84     | 0.14                | 0.86       |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 10                  | 0.84     | 0.29                | 0.92       |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 10                  | 0.8      | 0.16                | 0.86       |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 10                  | 0.8      | 0.23                | 0.79       |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 10                  | 0.8      | 0.23                | 0.79       |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 10                  | 0.8      | 0.23                | 0.79       |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 10                  | 0.79     | 0.21                | 0.76       |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 10                  | 0.79     | 0.25                | 0.68       |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 10                  | 0.78     | 0.22                | 0.84       |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 10                  | 0.78     | 0.13                | 0.74       |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 10                  | 0.77     | 0.24                | 0.78       |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 10                  | 0.76     | 0.22                | 0.7        |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 10                  | 0.75     | 0.27                | 0.65       |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 10                  | 0.75     | 0.27                | 0.65       |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 10                  | 0.75     | 0.27                | 0.65       |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 10                  | 0.75     | 0.27                | 0.65       |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 10                  | 0.75     | 0.27                | 0.65       |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 10                  | 0.75     | 0.27                | 0.65       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 10                  | 0.75     | 0.24                | 0.84       |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 10                  | 0.74     | 0.27                | 0.8        |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 10                  | 0.74     | 0.27                | 0.8        |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 10                  | 0.74     | 0.27                | 0.8        |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 10                  | 0.74     | 0.19                | 0.76       |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 10                  | 0.74     | 0.19                | 0.76       |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 10                  | 0.74     | 0.19                | 0.76       |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 10                  | 0.72     | 0.58                | 0.4        |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 10                  | 0.72     | 0.13                | 0.7        |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 10                  | 0.72     | 0.13                | 0.7        |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 10                  | 0.72     | 0.13                | 0.7        |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 10                  | 0.71     | 0.15                | 0.76       |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 10                  | 0.71     | 0.15                | 0.76       |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 10                  | 0.71     | 0.15                | 0.76       |
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 10                  | 0.69     | 0.04                | 0.68       |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 10                  | 0.69     | 0.38                | 0.55       |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 10                  | 0.68     | 0.1                 | 0.71       |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 10                  | 0.67     | 0.34                | 0.59       |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 10                  | 0.67     | 0.34                | 0.59       |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 10                  | 0.67     | 0.34                | 0.59       |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 10                  | 0.67     | 0.33                | 0.62       |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 10                  | 0.66     | 0.18                | 0.7        |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 10                  | 0.64     | 0.26                | 0.63       |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 10                  | 0.64     | 0.15                | 0.64       |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG22 | 10                  | 0.63     | 0.06                | 0.66       |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG21 | 10                  | 0.63     | 0.06                | 0.66       |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG23 | 10                  | 0.63     | 0.06                | 0.66       |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HD11 | 10                  | 0.63     | 0.06                | 0.66       |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HD13 | 10                  | 0.63     | 0.06                | 0.66       |
| (1,958)  | 1:145:A:PRO:HG3  | 1:146:A:PRO:HD2  | 10                  | 0.62     | 0.12                | 0.66       |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 10                  | 0.61     | 0.13                | 0.6        |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 10                  | 0.61     | 0.13                | 0.6        |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 10                  | 0.61     | 0.13                | 0.6        |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 10                  | 0.61     | 0.16                | 0.64       |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 10                  | 0.61     | 0.16                | 0.64       |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 10                  | 0.61     | 0.16                | 0.64       |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 10                  | 0.61     | 0.32                | 0.5        |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 10                  | 0.6      | 0.18                | 0.67       |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 10                  | 0.6      | 0.18                | 0.67       |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 10                  | 0.6      | 0.18                | 0.67       |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 10                  | 0.6      | 0.1                 | 0.6        |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 10                  | 0.6      | 0.1                 | 0.6        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 10                  | 0.6      | 0.1                 | 0.6        |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 10                  | 0.6      | 0.2                 | 0.6        |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 10                  | 0.58     | 0.11                | 0.6        |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB3   | 10                  | 0.58     | 0.11                | 0.6        |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 10                  | 0.57     | 0.24                | 0.47       |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB3   | 10                  | 0.56     | 0.08                | 0.55       |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 10                  | 0.56     | 0.08                | 0.55       |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 10                  | 0.55     | 0.31                | 0.48       |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 10                  | 0.55     | 0.14                | 0.58       |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 10                  | 0.54     | 0.23                | 0.61       |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 10                  | 0.54     | 0.2                 | 0.54       |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 10                  | 0.54     | 0.08                | 0.53       |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 10                  | 0.52     | 0.17                | 0.48       |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 10                  | 0.52     | 0.15                | 0.58       |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 10                  | 0.51     | 0.17                | 0.46       |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 10                  | 0.5      | 0.21                | 0.45       |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 10                  | 0.5      | 0.01                | 0.5        |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG22 | 10                  | 0.49     | 0.09                | 0.48       |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG23 | 10                  | 0.49     | 0.09                | 0.48       |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG21 | 10                  | 0.49     | 0.09                | 0.48       |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 10                  | 0.49     | 0.02                | 0.48       |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 10                  | 0.48     | 0.2                 | 0.52       |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD11 | 10                  | 0.48     | 0.12                | 0.51       |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD12 | 10                  | 0.48     | 0.12                | 0.51       |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD13 | 10                  | 0.48     | 0.12                | 0.51       |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD21 | 10                  | 0.48     | 0.12                | 0.51       |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD22 | 10                  | 0.48     | 0.12                | 0.51       |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD23 | 10                  | 0.48     | 0.12                | 0.51       |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 10                  | 0.48     | 0.1                 | 0.48       |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 10                  | 0.48     | 0.2                 | 0.54       |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 10                  | 0.48     | 0.13                | 0.54       |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 10                  | 0.48     | 0.13                | 0.54       |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 10                  | 0.48     | 0.13                | 0.54       |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 10                  | 0.47     | 0.15                | 0.52       |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 10                  | 0.47     | 0.15                | 0.52       |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 10                  | 0.47     | 0.15                | 0.52       |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 10                  | 0.46     | 0.06                | 0.48       |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 10                  | 0.46     | 0.06                | 0.48       |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 10                  | 0.46     | 0.06                | 0.48       |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 10                  | 0.46     | 0.15                | 0.44       |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 10                  | 0.45     | 0.06                | 0.43       |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 10                  | 0.44     | 0.19                | 0.5        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 10                  | 0.44     | 0.05                | 0.46       |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD3   | 10                  | 0.44     | 0.17                | 0.4        |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD2   | 10                  | 0.44     | 0.17                | 0.4        |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 10                  | 0.44     | 0.15                | 0.5        |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 10                  | 0.44     | 0.15                | 0.5        |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 10                  | 0.44     | 0.15                | 0.5        |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 10                  | 0.43     | 0.04                | 0.42       |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 10                  | 0.43     | 0.1                 | 0.42       |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 10                  | 0.43     | 0.1                 | 0.42       |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 10                  | 0.43     | 0.1                 | 0.42       |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 10                  | 0.43     | 0.1                 | 0.42       |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD21 | 10                  | 0.43     | 0.1                 | 0.42       |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD22 | 10                  | 0.43     | 0.1                 | 0.42       |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD23 | 10                  | 0.43     | 0.1                 | 0.42       |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 10                  | 0.42     | 0.07                | 0.41       |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 10                  | 0.42     | 0.07                | 0.41       |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 10                  | 0.42     | 0.07                | 0.41       |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 10                  | 0.42     | 0.18                | 0.46       |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 10                  | 0.42     | 0.05                | 0.43       |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 10                  | 0.42     | 0.05                | 0.43       |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 10                  | 0.42     | 0.05                | 0.43       |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 10                  | 0.41     | 0.07                | 0.42       |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 10                  | 0.41     | 0.11                | 0.46       |
| (1,356)  | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 10                  | 0.41     | 0.04                | 0.4        |
| (1,930)  | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 10                  | 0.41     | 0.04                | 0.41       |
| (1,930)  | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 10                  | 0.41     | 0.04                | 0.41       |
| (1,930)  | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 10                  | 0.41     | 0.04                | 0.41       |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 10                  | 0.41     | 0.11                | 0.4        |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 10                  | 0.41     | 0.11                | 0.4        |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 10                  | 0.41     | 0.11                | 0.4        |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 10                  | 0.4      | 0.06                | 0.4        |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 10                  | 0.4      | 0.06                | 0.4        |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 10                  | 0.4      | 0.06                | 0.4        |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 10                  | 0.39     | 0.02                | 0.4        |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 10                  | 0.39     | 0.02                | 0.4        |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 10                  | 0.39     | 0.02                | 0.4        |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 10                  | 0.39     | 0.1                 | 0.4        |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 10                  | 0.38     | 0.07                | 0.41       |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 10                  | 0.38     | 0.07                | 0.41       |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 10                  | 0.38     | 0.07                | 0.41       |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 10                  | 0.38     | 0.07                | 0.38       |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 10                  | 0.38     | 0.07                | 0.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 10                  | 0.38     | 0.07                | 0.38       |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 10                  | 0.38     | 0.03                | 0.38       |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 10                  | 0.38     | 0.15                | 0.36       |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 10                  | 0.38     | 0.12                | 0.36       |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 10                  | 0.38     | 0.12                | 0.36       |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 10                  | 0.38     | 0.12                | 0.36       |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 10                  | 0.38     | 0.13                | 0.36       |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 10                  | 0.36     | 0.16                | 0.38       |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 10                  | 0.36     | 0.03                | 0.36       |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 10                  | 0.36     | 0.2                 | 0.24       |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 10                  | 0.36     | 0.2                 | 0.24       |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 10                  | 0.36     | 0.2                 | 0.24       |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 10                  | 0.35     | 0.08                | 0.35       |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 10                  | 0.35     | 0.1                 | 0.36       |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 10                  | 0.35     | 0.16                | 0.34       |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 10                  | 0.34     | 0.07                | 0.36       |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 10                  | 0.34     | 0.13                | 0.36       |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 10                  | 0.34     | 0.13                | 0.36       |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 10                  | 0.34     | 0.13                | 0.36       |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 10                  | 0.34     | 0.06                | 0.33       |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 10                  | 0.33     | 0.03                | 0.34       |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 10                  | 0.32     | 0.02                | 0.34       |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 10                  | 0.32     | 0.04                | 0.32       |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 10                  | 0.32     | 0.04                | 0.32       |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 10                  | 0.32     | 0.04                | 0.32       |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 10                  | 0.32     | 0.06                | 0.31       |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 10                  | 0.32     | 0.06                | 0.31       |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 10                  | 0.32     | 0.06                | 0.31       |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 10                  | 0.32     | 0.07                | 0.29       |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 10                  | 0.32     | 0.07                | 0.29       |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 10                  | 0.32     | 0.07                | 0.29       |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 10                  | 0.3      | 0.03                | 0.3        |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 10                  | 0.29     | 0.11                | 0.29       |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 10                  | 0.29     | 0.11                | 0.29       |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 10                  | 0.29     | 0.11                | 0.29       |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 10                  | 0.29     | 0.04                | 0.3        |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 10                  | 0.29     | 0.04                | 0.28       |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 10                  | 0.29     | 0.04                | 0.28       |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 10                  | 0.29     | 0.04                | 0.28       |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 10                  | 0.29     | 0.07                | 0.29       |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 10                  | 0.29     | 0.07                | 0.29       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 10                  | 0.29     | 0.07                | 0.29       |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 10                  | 0.28     | 0.09                | 0.3        |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 10                  | 0.28     | 0.09                | 0.3        |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 10                  | 0.28     | 0.09                | 0.3        |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 10                  | 0.28     | 0.1                 | 0.28       |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 10                  | 0.27     | 0.03                | 0.28       |
| (1,359)  | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 10                  | 0.27     | 0.1                 | 0.24       |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 10                  | 0.27     | 0.1                 | 0.28       |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 10                  | 0.26     | 0.08                | 0.29       |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 10                  | 0.26     | 0.08                | 0.29       |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 10                  | 0.26     | 0.08                | 0.29       |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 10                  | 0.25     | 0.1                 | 0.24       |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 10                  | 0.25     | 0.07                | 0.25       |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG2  | 10                  | 0.25     | 0.07                | 0.25       |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 10                  | 0.25     | 0.05                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 10                  | 0.25     | 0.12                | 0.21       |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 10                  | 0.24     | 0.04                | 0.24       |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 10                  | 0.24     | 0.04                | 0.24       |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 10                  | 0.24     | 0.04                | 0.24       |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 10                  | 0.24     | 0.02                | 0.25       |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 10                  | 0.23     | 0.07                | 0.2        |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 10                  | 0.23     | 0.02                | 0.24       |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 10                  | 0.23     | 0.02                | 0.24       |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 10                  | 0.23     | 0.02                | 0.24       |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 10                  | 0.23     | 0.05                | 0.22       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 10                  | 0.23     | 0.07                | 0.2        |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 10                  | 0.23     | 0.06                | 0.23       |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 10                  | 0.22     | 0.04                | 0.24       |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 10                  | 0.22     | 0.04                | 0.24       |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 10                  | 0.22     | 0.04                | 0.24       |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 10                  | 0.22     | 0.02                | 0.22       |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 10                  | 0.22     | 0.03                | 0.22       |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 10                  | 0.22     | 0.03                | 0.22       |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 10                  | 0.22     | 0.03                | 0.22       |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 10                  | 0.21     | 0.02                | 0.2        |
| (1,349)  | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 10                  | 0.21     | 0.02                | 0.21       |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 10                  | 0.2      | 0.01                | 0.2        |
| (1,306)  | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 10                  | 0.2      | 0.01                | 0.2        |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 10                  | 0.2      | 0.06                | 0.2        |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 10                  | 0.2      | 0.06                | 0.2        |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 10                  | 0.2      | 0.06                | 0.2        |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 10                  | 0.19     | 0.04                | 0.2        |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 10                  | 0.19     | 0.02                | 0.18       |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 10                  | 0.19     | 0.02                | 0.18       |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 10                  | 0.19     | 0.02                | 0.18       |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 10                  | 0.18     | 0.07                | 0.16       |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 10                  | 0.18     | 0.07                | 0.16       |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 10                  | 0.18     | 0.07                | 0.16       |
| (1,283)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 10                  | 0.18     | 0.04                | 0.2        |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 10                  | 0.18     | 0.05                | 0.18       |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG3  | 10                  | 0.18     | 0.05                | 0.18       |
| (1,842)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 10                  | 0.18     | 0.05                | 0.19       |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG21 | 10                  | 0.18     | 0.03                | 0.17       |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG22 | 10                  | 0.18     | 0.03                | 0.17       |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG23 | 10                  | 0.18     | 0.03                | 0.17       |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 10                  | 0.17     | 0.03                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 10                  | 0.17     | 0.03                | 0.16       |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 10                  | 0.16     | 0.01                | 0.16       |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 10                  | 0.16     | 0.01                | 0.16       |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,4192) | 1:161:B:GLY:H    | 1:161:B:GLY:HA2  | 10                  | 0.15     | 0.03                | 0.15       |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 10                  | 0.14     | 0.02                | 0.14       |
| (1,4283) | 1:169:B:MET:H    | 1:171:B:LYS:HE2  | 9                   | 3.05     | 1.55                | 3.0        |
| (1,4283) | 1:169:B:MET:H    | 1:171:B:LYS:HE3  | 9                   | 3.05     | 1.55                | 3.0        |
| (1,1302) | 1:169:A:MET:HB2  | 1:171:A:LYS:HE3  | 9                   | 2.24     | 1.38                | 2.07       |
| (1,1302) | 1:169:A:MET:HB2  | 1:171:A:LYS:HE2  | 9                   | 2.24     | 1.38                | 2.07       |
| (1,2298) | 1:93:B:ASP:HA    | 1:169:B:MET:HG2  | 9                   | 1.69     | 0.55                | 1.65       |
| (1,2285) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB3   | 9                   | 1.42     | 0.6                 | 1.53       |
| (1,2285) | 1:89:B:ARG:HB2   | 1:90:B:HIS:HB3   | 9                   | 1.42     | 0.6                 | 1.53       |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 9                   | 1.24     | 0.16                | 1.25       |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 9                   | 1.07     | 0.63                | 0.67       |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 9                   | 1.07     | 0.63                | 0.67       |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 9                   | 1.07     | 0.63                | 0.67       |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 9                   | 1.05     | 0.29                | 0.9        |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 9                   | 1.05     | 0.29                | 0.9        |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 9                   | 1.05     | 0.29                | 0.9        |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 9                   | 1.05     | 0.29                | 0.9        |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 9                   | 1.05     | 0.29                | 0.9        |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 9                   | 1.05     | 0.29                | 0.9        |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 9                   | 1.0      | 0.47                | 0.95       |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 9                   | 0.94     | 0.44                | 0.85       |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 9                   | 0.92     | 0.33                | 0.92       |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 9                   | 0.91     | 0.5                 | 0.79       |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 9                   | 0.86     | 0.3                 | 0.86       |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 9                   | 0.77     | 0.22                | 0.84       |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG22 | 9                   | 0.75     | 0.17                | 0.72       |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG21 | 9                   | 0.75     | 0.17                | 0.72       |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG23 | 9                   | 0.75     | 0.17                | 0.72       |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 9                   | 0.73     | 0.07                | 0.76       |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 9                   | 0.73     | 0.31                | 0.76       |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 9                   | 0.72     | 0.23                | 0.72       |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 9                   | 0.72     | 0.23                | 0.72       |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 9                   | 0.72     | 0.23                | 0.72       |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 9                   | 0.72     | 0.23                | 0.72       |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 9                   | 0.72     | 0.23                | 0.72       |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 9                   | 0.72     | 0.23                | 0.72       |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 9                   | 0.69     | 0.41                | 0.59       |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 9                   | 0.69     | 0.41                | 0.59       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 9                   | 0.66     | 0.31                | 0.6        |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 9                   | 0.61     | 0.29                | 0.61       |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG2  | 9                   | 0.61     | 0.29                | 0.61       |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 9                   | 0.59     | 0.22                | 0.65       |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 9                   | 0.59     | 0.22                | 0.65       |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 9                   | 0.59     | 0.22                | 0.65       |
| (1,2976) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB2  | 9                   | 0.59     | 0.2                 | 0.43       |
| (1,2976) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HB2  | 9                   | 0.59     | 0.2                 | 0.43       |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 9                   | 0.56     | 0.08                | 0.56       |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 9                   | 0.55     | 0.19                | 0.58       |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 9                   | 0.55     | 0.19                | 0.58       |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 9                   | 0.55     | 0.19                | 0.58       |
| (1,453)  | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 9                   | 0.54     | 0.39                | 0.33       |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 9                   | 0.54     | 0.16                | 0.56       |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 9                   | 0.53     | 0.15                | 0.56       |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 9                   | 0.52     | 0.25                | 0.57       |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 9                   | 0.52     | 0.25                | 0.57       |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 9                   | 0.52     | 0.25                | 0.57       |
| (1,71)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB2  | 9                   | 0.51     | 0.15                | 0.43       |
| (1,71)   | 1:95:A:TRP:HB2   | 1:168:A:PRO:HB2  | 9                   | 0.51     | 0.15                | 0.43       |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 9                   | 0.51     | 0.17                | 0.51       |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 9                   | 0.51     | 0.17                | 0.51       |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 9                   | 0.51     | 0.17                | 0.51       |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 9                   | 0.51     | 0.07                | 0.53       |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 9                   | 0.48     | 0.06                | 0.45       |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 9                   | 0.45     | 0.14                | 0.47       |
| (1,695)  | 1:123:A:LYS:HD2  | 1:137:A:CYS:HB2  | 9                   | 0.44     | 0.16                | 0.42       |
| (1,695)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HB2  | 9                   | 0.44     | 0.16                | 0.42       |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 9                   | 0.42     | 0.17                | 0.42       |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 9                   | 0.4      | 0.06                | 0.42       |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 9                   | 0.4      | 0.06                | 0.42       |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 9                   | 0.4      | 0.06                | 0.42       |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 9                   | 0.4      | 0.06                | 0.42       |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 9                   | 0.4      | 0.06                | 0.42       |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 9                   | 0.4      | 0.06                | 0.42       |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD3  | 9                   | 0.4      | 0.17                | 0.31       |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD2  | 9                   | 0.4      | 0.17                | 0.31       |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 9                   | 0.39     | 0.19                | 0.42       |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 9                   | 0.39     | 0.19                | 0.42       |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 9                   | 0.39     | 0.19                | 0.42       |
| (1,2352) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB2  | 9                   | 0.39     | 0.24                | 0.31       |
| (1,2352) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB2  | 9                   | 0.39     | 0.24                | 0.31       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 9                   | 0.38     | 0.13                | 0.38       |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 9                   | 0.38     | 0.03                | 0.39       |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 9                   | 0.38     | 0.03                | 0.39       |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 9                   | 0.38     | 0.03                | 0.39       |
| (1,694)  | 1:123:A:LYS:HD2  | 1:137:A:CYS:HA   | 9                   | 0.37     | 0.11                | 0.41       |
| (1,694)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HA   | 9                   | 0.37     | 0.11                | 0.41       |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 9                   | 0.37     | 0.08                | 0.4        |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 9                   | 0.37     | 0.08                | 0.4        |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 9                   | 0.37     | 0.08                | 0.4        |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 9                   | 0.36     | 0.12                | 0.38       |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 9                   | 0.35     | 0.11                | 0.37       |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 9                   | 0.35     | 0.14                | 0.37       |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 9                   | 0.35     | 0.2                 | 0.33       |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 9                   | 0.35     | 0.12                | 0.29       |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 9                   | 0.35     | 0.13                | 0.34       |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 9                   | 0.35     | 0.13                | 0.34       |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 9                   | 0.35     | 0.13                | 0.34       |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD11 | 9                   | 0.35     | 0.1                 | 0.36       |
| (1,1408) | 1:107:A:ASP:H    | 1:157:A:LEU:HD12 | 9                   | 0.35     | 0.1                 | 0.36       |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD13 | 9                   | 0.35     | 0.1                 | 0.36       |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD12 | 9                   | 0.35     | 0.1                 | 0.36       |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 9                   | 0.34     | 0.19                | 0.23       |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 9                   | 0.34     | 0.19                | 0.23       |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 9                   | 0.34     | 0.19                | 0.23       |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 9                   | 0.34     | 0.09                | 0.27       |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 9                   | 0.34     | 0.09                | 0.27       |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 9                   | 0.34     | 0.09                | 0.27       |
| (1,509)  | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 9                   | 0.33     | 0.15                | 0.38       |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 9                   | 0.33     | 0.15                | 0.32       |
| (1,72)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB3  | 9                   | 0.33     | 0.15                | 0.25       |
| (1,72)   | 1:95:A:TRP:HB2   | 1:168:A:PRO:HB3  | 9                   | 0.33     | 0.15                | 0.25       |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 9                   | 0.32     | 0.1                 | 0.27       |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 9                   | 0.32     | 0.1                 | 0.27       |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 9                   | 0.32     | 0.1                 | 0.27       |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 9                   | 0.32     | 0.09                | 0.31       |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 9                   | 0.32     | 0.09                | 0.31       |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 9                   | 0.32     | 0.09                | 0.31       |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 9                   | 0.3      | 0.19                | 0.18       |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 9                   | 0.3      | 0.19                | 0.18       |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 9                   | 0.3      | 0.19                | 0.18       |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD22 | 9                   | 0.29     | 0.08                | 0.24       |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD21 | 9                   | 0.29     | 0.08                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE3  | 9                   | 0.29     | 0.16                | 0.22       |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE2  | 9                   | 0.29     | 0.16                | 0.22       |
| (1,256)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 9                   | 0.29     | 0.06                | 0.29       |
| (1,256)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 9                   | 0.29     | 0.06                | 0.29       |
| (1,256)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 9                   | 0.29     | 0.06                | 0.29       |
| (1,383)  | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 9                   | 0.29     | 0.09                | 0.3        |
| (1,383)  | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 9                   | 0.29     | 0.09                | 0.3        |
| (1,383)  | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 9                   | 0.29     | 0.09                | 0.3        |
| (1,418)  | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 9                   | 0.28     | 0.11                | 0.25       |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 9                   | 0.27     | 0.07                | 0.23       |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 9                   | 0.27     | 0.06                | 0.26       |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 9                   | 0.26     | 0.07                | 0.28       |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 9                   | 0.25     | 0.05                | 0.26       |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 9                   | 0.25     | 0.15                | 0.15       |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 9                   | 0.24     | 0.07                | 0.24       |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 9                   | 0.24     | 0.12                | 0.2        |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 9                   | 0.24     | 0.12                | 0.2        |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 9                   | 0.24     | 0.12                | 0.2        |
| (1,639)  | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 9                   | 0.24     | 0.1                 | 0.26       |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 9                   | 0.22     | 0.07                | 0.21       |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 9                   | 0.22     | 0.04                | 0.23       |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 9                   | 0.21     | 0.07                | 0.22       |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 9                   | 0.21     | 0.07                | 0.22       |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 9                   | 0.21     | 0.07                | 0.22       |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 9                   | 0.21     | 0.07                | 0.22       |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 9                   | 0.21     | 0.07                | 0.22       |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 9                   | 0.21     | 0.07                | 0.22       |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 9                   | 0.21     | 0.02                | 0.21       |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 9                   | 0.21     | 0.09                | 0.18       |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 9                   | 0.21     | 0.09                | 0.18       |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 9                   | 0.21     | 0.09                | 0.18       |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD11  | 9                   | 0.21     | 0.03                | 0.2        |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD12  | 9                   | 0.21     | 0.03                | 0.2        |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD13  | 9                   | 0.21     | 0.03                | 0.2        |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD21  | 9                   | 0.21     | 0.03                | 0.2        |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD22  | 9                   | 0.21     | 0.03                | 0.2        |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD23  | 9                   | 0.21     | 0.03                | 0.2        |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 9                   | 0.2      | 0.02                | 0.21       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 9                   | 0.2      | 0.02                | 0.21       |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 9                   | 0.19     | 0.04                | 0.18       |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 9                   | 0.18     | 0.05                | 0.18       |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 9                   | 0.17     | 0.02                | 0.17       |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 9                   | 0.17     | 0.04                | 0.17       |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 9                   | 0.17     | 0.04                | 0.17       |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 9                   | 0.17     | 0.04                | 0.17       |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 9                   | 0.16     | 0.04                | 0.15       |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 9                   | 0.16     | 0.04                | 0.13       |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 9                   | 0.15     | 0.05                | 0.14       |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 9                   | 0.15     | 0.05                | 0.14       |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 9                   | 0.15     | 0.05                | 0.14       |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 9                   | 0.14     | 0.03                | 0.15       |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 9                   | 0.14     | 0.03                | 0.15       |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 9                   | 0.14     | 0.03                | 0.15       |
| (1,551)  | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 9                   | 0.14     | 0.02                | 0.14       |
| (1,551)  | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 9                   | 0.14     | 0.02                | 0.14       |
| (1,551)  | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 9                   | 0.14     | 0.02                | 0.14       |
| (1,2003) | 1:171:A:LYS:H    | 1:92:A:ALA:HB1   | 8                   | 4.5      | 1.66                | 4.6        |
| (1,2003) | 1:171:A:LYS:H    | 1:92:A:ALA:HB2   | 8                   | 4.5      | 1.66                | 4.6        |
| (1,2003) | 1:171:A:LYS:H    | 1:92:A:ALA:HB3   | 8                   | 4.5      | 1.66                | 4.6        |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB1   | 8                   | 4.42     | 1.88                | 4.83       |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB2   | 8                   | 4.42     | 1.88                | 4.83       |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB3   | 8                   | 4.42     | 1.88                | 4.83       |
| (1,3583) | 1:169:B:MET:HB2  | 1:171:B:LYS:HE3  | 8                   | 3.5      | 1.16                | 3.49       |
| (1,3583) | 1:169:B:MET:HB2  | 1:171:B:LYS:HE2  | 8                   | 3.5      | 1.16                | 3.49       |
| (1,3582) | 1:169:B:MET:HB3  | 1:171:B:LYS:HG3  | 8                   | 2.7      | 0.5                 | 2.6        |
| (1,3582) | 1:169:B:MET:HB3  | 1:171:B:LYS:HG2  | 8                   | 2.7      | 0.5                 | 2.6        |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 8                   | 1.4      | 0.52                | 1.62       |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 8                   | 1.4      | 0.52                | 1.62       |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 8                   | 1.4      | 0.52                | 1.62       |
| (1,3)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB2   | 8                   | 1.3      | 0.43                | 1.36       |
| (1,3)    | 1:89:A:ARG:HB2   | 1:90:A:HIS:HB2   | 8                   | 1.3      | 0.43                | 1.36       |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 8                   | 1.09     | 0.37                | 1.2        |
| (1,2284) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB2   | 8                   | 1.02     | 0.66                | 0.92       |
| (1,2284) | 1:89:B:ARG:HB2   | 1:90:B:HIS:HB2   | 8                   | 1.02     | 0.66                | 0.92       |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 8                   | 0.91     | 0.5                 | 0.94       |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 8                   | 0.7      | 0.19                | 0.78       |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 8                   | 0.65     | 0.28                | 0.74       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 8                   | 0.64     | 0.3                 | 0.75       |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG23 | 8                   | 0.64     | 0.19                | 0.55       |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG21 | 8                   | 0.64     | 0.19                | 0.55       |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG22 | 8                   | 0.64     | 0.19                | 0.55       |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 8                   | 0.61     | 0.22                | 0.6        |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 8                   | 0.61     | 0.22                | 0.6        |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG21 | 8                   | 0.57     | 0.27                | 0.6        |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG22 | 8                   | 0.57     | 0.27                | 0.6        |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG23 | 8                   | 0.57     | 0.27                | 0.6        |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 8                   | 0.56     | 0.25                | 0.6        |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 8                   | 0.56     | 0.25                | 0.6        |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 8                   | 0.55     | 0.3                 | 0.48       |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 8                   | 0.55     | 0.3                 | 0.48       |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 8                   | 0.55     | 0.3                 | 0.48       |
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 8                   | 0.54     | 0.19                | 0.56       |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 8                   | 0.54     | 0.24                | 0.54       |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 8                   | 0.52     | 0.28                | 0.42       |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 8                   | 0.5      | 0.18                | 0.44       |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 8                   | 0.5      | 0.23                | 0.5        |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 8                   | 0.5      | 0.15                | 0.56       |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 8                   | 0.48     | 0.39                | 0.3        |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 8                   | 0.48     | 0.39                | 0.3        |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 8                   | 0.48     | 0.39                | 0.3        |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD21 | 8                   | 0.47     | 0.11                | 0.51       |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD22 | 8                   | 0.47     | 0.11                | 0.51       |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD23 | 8                   | 0.47     | 0.11                | 0.51       |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 8                   | 0.41     | 0.09                | 0.41       |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 8                   | 0.41     | 0.09                | 0.41       |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 8                   | 0.41     | 0.09                | 0.41       |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD2   | 8                   | 0.4      | 0.12                | 0.43       |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD3   | 8                   | 0.4      | 0.12                | 0.43       |
| (1,3378) | 1:154:B:SER:HB3  | 1:155:B:SER:HA   | 8                   | 0.39     | 0.12                | 0.44       |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 8                   | 0.37     | 0.17                | 0.44       |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 8                   | 0.36     | 0.11                | 0.35       |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 8                   | 0.36     | 0.11                | 0.35       |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 8                   | 0.36     | 0.11                | 0.35       |
| (1,2975) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HA   | 8                   | 0.35     | 0.09                | 0.31       |
| (1,2975) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HA   | 8                   | 0.35     | 0.09                | 0.31       |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD11 | 8                   | 0.34     | 0.13                | 0.37       |
| (1,3689) | 1:107:B:ASP:H    | 1:157:B:LEU:HD13 | 8                   | 0.34     | 0.13                | 0.37       |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD12 | 8                   | 0.34     | 0.13                | 0.37       |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD13 | 8                   | 0.34     | 0.13                | 0.37       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 8                   | 0.34     | 0.07                | 0.36       |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 8                   | 0.33     | 0.19                | 0.26       |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 8                   | 0.32     | 0.06                | 0.32       |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 8                   | 0.32     | 0.06                | 0.32       |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 8                   | 0.32     | 0.06                | 0.32       |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 8                   | 0.32     | 0.15                | 0.28       |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 8                   | 0.32     | 0.15                | 0.28       |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 8                   | 0.32     | 0.15                | 0.28       |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 8                   | 0.32     | 0.16                | 0.24       |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 8                   | 0.32     | 0.16                | 0.24       |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 8                   | 0.32     | 0.16                | 0.24       |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD22 | 8                   | 0.32     | 0.09                | 0.3        |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD21 | 8                   | 0.32     | 0.09                | 0.3        |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 8                   | 0.31     | 0.16                | 0.31       |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 8                   | 0.31     | 0.1                 | 0.32       |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 8                   | 0.31     | 0.1                 | 0.32       |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 8                   | 0.31     | 0.1                 | 0.32       |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 8                   | 0.31     | 0.1                 | 0.32       |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 8                   | 0.31     | 0.1                 | 0.32       |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 8                   | 0.31     | 0.1                 | 0.32       |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 8                   | 0.31     | 0.16                | 0.26       |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 8                   | 0.31     | 0.16                | 0.26       |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 8                   | 0.31     | 0.16                | 0.26       |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 8                   | 0.31     | 0.16                | 0.26       |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 8                   | 0.31     | 0.16                | 0.26       |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 8                   | 0.31     | 0.16                | 0.26       |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 8                   | 0.3      | 0.14                | 0.3        |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 8                   | 0.28     | 0.11                | 0.3        |
| (1,280)  | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA3  | 8                   | 0.27     | 0.14                | 0.21       |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 8                   | 0.27     | 0.11                | 0.24       |
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 8                   | 0.27     | 0.11                | 0.24       |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 8                   | 0.27     | 0.11                | 0.24       |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 8                   | 0.26     | 0.08                | 0.3        |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 8                   | 0.25     | 0.07                | 0.28       |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 8                   | 0.24     | 0.13                | 0.2        |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 8                   | 0.24     | 0.13                | 0.2        |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 8                   | 0.24     | 0.13                | 0.2        |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 8                   | 0.24     | 0.06                | 0.26       |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 8                   | 0.24     | 0.06                | 0.26       |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 8                   | 0.24     | 0.06                | 0.26       |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 8                   | 0.23     | 0.14                | 0.18       |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 8                   | 0.22     | 0.05                | 0.22       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3726) | 1:111:B:VAL:H    | 1:110:B:THR:HB   | 8                   | 0.2      | 0.07                | 0.22       |
| (1,647)  | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 8                   | 0.2      | 0.08                | 0.2        |
| (1,647)  | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 8                   | 0.2      | 0.08                | 0.2        |
| (1,647)  | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 8                   | 0.2      | 0.08                | 0.2        |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 8                   | 0.19     | 0.03                | 0.2        |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG11 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG12 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG13 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG11 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG12 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG13 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG11 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG12 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG13 | 8                   | 0.18     | 0.05                | 0.19       |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 8                   | 0.18     | 0.03                | 0.18       |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 8                   | 0.18     | 0.05                | 0.18       |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 8                   | 0.17     | 0.06                | 0.16       |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 8                   | 0.17     | 0.06                | 0.16       |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 8                   | 0.17     | 0.06                | 0.16       |
| (1,521)  | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 8                   | 0.17     | 0.04                | 0.18       |
| (1,521)  | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 8                   | 0.17     | 0.04                | 0.18       |
| (1,521)  | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 8                   | 0.17     | 0.04                | 0.18       |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD11 | 8                   | 0.17     | 0.05                | 0.18       |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD12 | 8                   | 0.17     | 0.05                | 0.18       |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD13 | 8                   | 0.17     | 0.05                | 0.18       |
| (1,2326) | 1:94:B:ARG:HG2   | 1:168:B:PRO:HB2  | 8                   | 0.17     | 0.05                | 0.14       |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 8                   | 0.16     | 0.05                | 0.15       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 8                   | 0.16     | 0.05                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,371)  | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 8                   | 0.16     | 0.03                | 0.15       |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 8                   | 0.15     | 0.02                | 0.16       |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 8                   | 0.15     | 0.04                | 0.16       |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 8                   | 0.15     | 0.02                | 0.15       |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 8                   | 0.13     | 0.01                | 0.13       |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB1   | 7                   | 2.8      | 0.93                | 2.74       |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB2   | 7                   | 2.8      | 0.93                | 2.74       |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB3   | 7                   | 2.8      | 0.93                | 2.74       |
| (1,2002) | 1:169:A:MET:H    | 1:171:A:LYS:HE3  | 7                   | 2.74     | 1.52                | 2.35       |
| (1,2002) | 1:169:A:MET:H    | 1:171:A:LYS:HE2  | 7                   | 2.74     | 1.52                | 2.35       |
| (1,2)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HB3   | 7                   | 1.86     | 1.16                | 1.38       |
| (1,2)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HB3   | 7                   | 1.86     | 1.16                | 1.38       |
| (1,2)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HB3   | 7                   | 1.86     | 1.16                | 1.38       |
| (1,2283) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HB3   | 7                   | 1.53     | 0.92                | 1.58       |
| (1,2283) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HB3   | 7                   | 1.53     | 0.92                | 1.58       |
| (1,2283) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HB3   | 7                   | 1.53     | 0.92                | 1.58       |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG21  | 7                   | 1.22     | 1.02                | 1.37       |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG22  | 7                   | 1.22     | 1.02                | 1.37       |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG23  | 7                   | 1.22     | 1.02                | 1.37       |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 7                   | 0.99     | 0.28                | 1.14       |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 7                   | 0.99     | 0.28                | 1.14       |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB1  | 7                   | 0.93     | 0.11                | 0.96       |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB2  | 7                   | 0.93     | 0.11                | 0.96       |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB3  | 7                   | 0.93     | 0.11                | 0.96       |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 7                   | 0.89     | 0.23                | 0.99       |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 7                   | 0.89     | 0.23                | 0.99       |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 7                   | 0.76     | 0.31                | 0.84       |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1  | 7                   | 0.75     | 0.14                | 0.81       |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2  | 7                   | 0.75     | 0.14                | 0.81       |
| (1,4267) | 1:167:B:ALA:H    | 1:169:B:MET:H    | 7                   | 0.73     | 0.33                | 0.65       |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 7                   | 0.68     | 0.54                | 0.54       |
| (1,2282) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HA    | 7                   | 0.64     | 0.41                | 0.51       |
| (1,2282) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HA    | 7                   | 0.64     | 0.41                | 0.51       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2282) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HA    | 7                   | 0.64     | 0.41                | 0.51       |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 7                   | 0.61     | 0.26                | 0.67       |
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 7                   | 0.58     | 0.21                | 0.57       |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD2  | 7                   | 0.52     | 0.16                | 0.52       |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD3  | 7                   | 0.52     | 0.16                | 0.52       |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 7                   | 0.52     | 0.32                | 0.39       |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 7                   | 0.52     | 0.32                | 0.39       |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 7                   | 0.52     | 0.32                | 0.39       |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD3  | 7                   | 0.52     | 0.37                | 0.44       |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD2  | 7                   | 0.52     | 0.37                | 0.44       |
| (1,1654) | 1:134:A:ILE:H    | 1:127:A:ARG:HB2  | 7                   | 0.45     | 0.43                | 0.3        |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 7                   | 0.41     | 0.13                | 0.31       |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 7                   | 0.41     | 0.13                | 0.31       |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 7                   | 0.41     | 0.13                | 0.31       |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 7                   | 0.4      | 0.15                | 0.5        |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 7                   | 0.4      | 0.24                | 0.28       |
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 7                   | 0.38     | 0.13                | 0.44       |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG3  | 7                   | 0.37     | 0.21                | 0.29       |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG2  | 7                   | 0.37     | 0.21                | 0.29       |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 7                   | 0.34     | 0.22                | 0.2        |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 7                   | 0.34     | 0.11                | 0.35       |
| (1,2353) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB3  | 7                   | 0.34     | 0.21                | 0.28       |
| (1,2353) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB3  | 7                   | 0.34     | 0.21                | 0.28       |
| (1,4197) | 1:162:B:THR:H    | 1:102:B:ASN:HB3  | 7                   | 0.34     | 0.23                | 0.32       |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 7                   | 0.33     | 0.07                | 0.37       |
| (1,1193) | 1:158:A:SER:HB3  | 1:160:A:GLU:HB3  | 7                   | 0.32     | 0.14                | 0.34       |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 7                   | 0.3      | 0.08                | 0.28       |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 7                   | 0.28     | 0.08                | 0.29       |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 7                   | 0.28     | 0.08                | 0.29       |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 7                   | 0.28     | 0.08                | 0.29       |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 7                   | 0.27     | 0.09                | 0.3        |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 7                   | 0.27     | 0.09                | 0.3        |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 7                   | 0.27     | 0.09                | 0.3        |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 7                   | 0.27     | 0.07                | 0.28       |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 7                   | 0.26     | 0.05                | 0.23       |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 7                   | 0.26     | 0.08                | 0.25       |
| (1,102)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HB3  | 7                   | 0.26     | 0.07                | 0.28       |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 7                   | 0.24     | 0.03                | 0.25       |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 7                   | 0.24     | 0.03                | 0.25       |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 7                   | 0.24     | 0.03                | 0.25       |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 7                   | 0.24     | 0.14                | 0.22       |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 7                   | 0.22     | 0.09                | 0.22       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 7                   | 0.22     | 0.09                | 0.22       |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 7                   | 0.22     | 0.09                | 0.22       |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG21  | 7                   | 0.21     | 0.09                | 0.19       |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG22  | 7                   | 0.21     | 0.09                | 0.19       |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG23  | 7                   | 0.21     | 0.09                | 0.19       |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG21  | 7                   | 0.21     | 0.09                | 0.19       |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG22  | 7                   | 0.21     | 0.09                | 0.19       |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG23  | 7                   | 0.21     | 0.09                | 0.19       |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 7                   | 0.21     | 0.05                | 0.19       |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 7                   | 0.21     | 0.05                | 0.19       |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 7                   | 0.21     | 0.05                | 0.19       |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 7                   | 0.19     | 0.06                | 0.19       |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 7                   | 0.19     | 0.06                | 0.19       |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 7                   | 0.19     | 0.06                | 0.19       |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG21 | 7                   | 0.18     | 0.06                | 0.15       |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG22 | 7                   | 0.18     | 0.06                | 0.15       |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG23 | 7                   | 0.18     | 0.06                | 0.15       |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 7                   | 0.18     | 0.07                | 0.15       |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD21  | 7                   | 0.16     | 0.04                | 0.15       |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD22  | 7                   | 0.16     | 0.04                | 0.15       |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD23  | 7                   | 0.16     | 0.04                | 0.15       |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD11  | 7                   | 0.16     | 0.04                | 0.15       |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD12  | 7                   | 0.16     | 0.04                | 0.15       |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD13  | 7                   | 0.16     | 0.04                | 0.15       |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD11 | 7                   | 0.16     | 0.03                | 0.16       |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD12 | 7                   | 0.16     | 0.03                | 0.16       |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD13 | 7                   | 0.16     | 0.03                | 0.16       |
| (1,1657) | 1:134:A:ILE:H    | 1:133:A:TYR:HB3  | 7                   | 0.16     | 0.04                | 0.14       |
| (1,3936) | 1:134:B:ILE:H    | 1:127:B:ARG:HG2  | 7                   | 0.16     | 0.04                | 0.15       |
| (1,680)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 7                   | 0.15     | 0.02                | 0.16       |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 7                   | 0.15     | 0.04                | 0.16       |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 7                   | 0.15     | 0.04                | 0.16       |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 7                   | 0.15     | 0.04                | 0.16       |
| (1,23)   | 1:94:A:ARG:HA    | 1:94:A:ARG:HB3   | 7                   | 0.15     | 0.03                | 0.13       |
| (1,502)  | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 7                   | 0.14     | 0.04                | 0.12       |
| (1,502)  | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 7                   | 0.14     | 0.04                | 0.12       |
| (1,502)  | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 7                   | 0.14     | 0.04                | 0.12       |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD1  | 7                   | 0.14     | 0.04                | 0.13       |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD2  | 7                   | 0.14     | 0.04                | 0.13       |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD1  | 7                   | 0.14     | 0.04                | 0.13       |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD2  | 7                   | 0.14     | 0.04                | 0.13       |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD1  | 7                   | 0.14     | 0.04                | 0.13       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD2  | 7                   | 0.14     | 0.04                | 0.13       |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 7                   | 0.13     | 0.03                | 0.12       |
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 7                   | 0.13     | 0.03                | 0.12       |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 7                   | 0.13     | 0.03                | 0.12       |
| (1,4034) | 1:148:B:VAL:H    | 1:149:B:ASP:H    | 7                   | 0.13     | 0.04                | 0.11       |
| (1,1)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HA    | 6                   | 1.22     | 0.81                | 0.8        |
| (1,1)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HA    | 6                   | 1.22     | 0.81                | 0.8        |
| (1,1)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HA    | 6                   | 1.22     | 0.81                | 0.8        |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD1  | 6                   | 1.18     | 0.49                | 1.25       |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD2  | 6                   | 1.18     | 0.49                | 1.25       |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD1  | 6                   | 1.01     | 0.4                 | 0.92       |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD2  | 6                   | 1.01     | 0.4                 | 0.92       |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG21  | 6                   | 0.98     | 0.57                | 0.84       |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG22  | 6                   | 0.98     | 0.57                | 0.84       |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG23  | 6                   | 0.98     | 0.57                | 0.84       |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE1  | 6                   | 0.97     | 0.08                | 0.98       |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE2  | 6                   | 0.97     | 0.08                | 0.98       |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE1  | 6                   | 0.97     | 0.08                | 0.98       |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE2  | 6                   | 0.97     | 0.08                | 0.98       |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE1  | 6                   | 0.97     | 0.08                | 0.98       |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE2  | 6                   | 0.97     | 0.08                | 0.98       |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE1  | 6                   | 0.97     | 0.26                | 0.96       |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE2  | 6                   | 0.97     | 0.26                | 0.96       |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB1  | 6                   | 0.95     | 0.66                | 0.72       |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB2  | 6                   | 0.95     | 0.66                | 0.72       |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB3  | 6                   | 0.95     | 0.66                | 0.72       |
| (1,2025) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 6                   | 0.84     | 0.48                | 0.89       |
| (1,2157) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 6                   | 0.84     | 0.48                | 0.89       |
| (1,990)  | 1:148:A:VAL:HA   | 1:169:A:MET:HB2  | 6                   | 0.75     | 0.32                | 0.85       |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE1  | 6                   | 0.72     | 0.34                | 0.83       |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE2  | 6                   | 0.72     | 0.34                | 0.83       |
| (1,1012) | 1:148:A:VAL:HG11 | 1:169:A:MET:HB2  | 6                   | 0.68     | 0.28                | 0.78       |
| (1,1012) | 1:148:A:VAL:HG12 | 1:169:A:MET:HB2  | 6                   | 0.68     | 0.28                | 0.78       |
| (1,1012) | 1:148:A:VAL:HG13 | 1:169:A:MET:HB2  | 6                   | 0.68     | 0.28                | 0.78       |
| (1,710)  | 1:126:A:GLU:HA   | 1:135:A:SER:HB2  | 6                   | 0.65     | 0.28                | 0.66       |
| (1,1916) | 1:162:A:THR:H    | 1:102:A:ASN:HB3  | 6                   | 0.63     | 0.21                | 0.58       |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG21 | 6                   | 0.63     | 0.08                | 0.64       |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG22 | 6                   | 0.63     | 0.08                | 0.64       |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG23 | 6                   | 0.63     | 0.08                | 0.64       |
| (1,722)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HA   | 6                   | 0.6      | 0.25                | 0.48       |
| (1,2907) | 1:120:B:ILE:HA   | 1:120:B:ILE:HG13 | 6                   | 0.55     | 0.03                | 0.54       |
| (1,688)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB3  | 6                   | 0.52     | 0.18                | 0.5        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB1  | 6                   | 0.49     | 0.26                | 0.6        |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB2  | 6                   | 0.49     | 0.26                | 0.6        |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB3  | 6                   | 0.49     | 0.26                | 0.6        |
| (1,684)  | 1:123:A:LYS:HA   | 1:135:A:SER:HB3  | 6                   | 0.48     | 0.3                 | 0.49       |
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 6                   | 0.47     | 0.13                | 0.51       |
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD3  | 6                   | 0.47     | 0.13                | 0.51       |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 6                   | 0.47     | 0.13                | 0.51       |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD3  | 6                   | 0.47     | 0.13                | 0.51       |
| (1,1998) | 1:169:A:MET:H    | 1:169:A:MET:HB2  | 6                   | 0.46     | 0.26                | 0.34       |
| (1,723)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB2  | 6                   | 0.44     | 0.16                | 0.5        |
| (1,3612) | 1:95:B:TRP:H     | 1:95:B:TRP:HB2   | 6                   | 0.44     | 0.05                | 0.43       |
| (1,827)  | 1:139:A:THR:HA   | 1:140:A:ARG:HG2  | 6                   | 0.43     | 0.26                | 0.28       |
| (1,99)   | 1:96:A:ARG:HB3   | 1:164:A:THR:HB   | 6                   | 0.43     | 0.16                | 0.37       |
| (1,3904) | 1:129:B:ASP:H    | 1:130:B:GLU:HG3  | 6                   | 0.43     | 0.16                | 0.42       |
| (1,3904) | 1:129:B:ASP:H    | 1:130:B:GLU:HG2  | 6                   | 0.43     | 0.16                | 0.42       |
| (1,2081) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 6                   | 0.43     | 0.22                | 0.38       |
| (1,2213) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 6                   | 0.43     | 0.22                | 0.38       |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE3  | 6                   | 0.41     | 0.21                | 0.4        |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE3  | 6                   | 0.41     | 0.21                | 0.4        |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE3  | 6                   | 0.41     | 0.21                | 0.4        |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE2  | 6                   | 0.41     | 0.21                | 0.4        |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE2  | 6                   | 0.41     | 0.21                | 0.4        |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE2  | 6                   | 0.41     | 0.21                | 0.4        |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG22 | 6                   | 0.39     | 0.2                 | 0.36       |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG23 | 6                   | 0.39     | 0.2                 | 0.36       |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG21 | 6                   | 0.39     | 0.2                 | 0.36       |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB1   | 6                   | 0.39     | 0.2                 | 0.47       |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB2   | 6                   | 0.39     | 0.2                 | 0.47       |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB3   | 6                   | 0.39     | 0.2                 | 0.47       |
| (1,3460) | 1:157:B:LEU:HD21 | 1:163:B:LEU:HB3  | 6                   | 0.38     | 0.11                | 0.42       |
| (1,3460) | 1:157:B:LEU:HD22 | 1:163:B:LEU:HB3  | 6                   | 0.38     | 0.11                | 0.42       |
| (1,3460) | 1:157:B:LEU:HD23 | 1:163:B:LEU:HB3  | 6                   | 0.38     | 0.11                | 0.42       |
| (1,3491) | 1:160:B:GLU:HB2  | 1:162:B:THR:HB   | 6                   | 0.38     | 0.12                | 0.38       |
| (1,3137) | 1:141:B:LYS:HG2  | 1:142:B:TYR:HB3  | 6                   | 0.38     | 0.11                | 0.37       |
| (1,2037) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 6                   | 0.35     | 0.11                | 0.34       |
| (1,2169) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 6                   | 0.35     | 0.11                | 0.34       |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG3  | 6                   | 0.35     | 0.2                 | 0.34       |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG2  | 6                   | 0.35     | 0.2                 | 0.34       |
| (1,2996) | 1:126:B:GLU:HB2  | 1:135:B:SER:HB3  | 6                   | 0.33     | 0.22                | 0.24       |
| (1,9)    | 1:90:A:HIS:HB3   | 1:91:A:THR:HA    | 6                   | 0.33     | 0.18                | 0.27       |
| (1,3847) | 1:123:B:LYS:H    | 1:109:B:LEU:HB2  | 6                   | 0.32     | 0.06                | 0.32       |
| (1,1210) | 1:160:A:GLU:HB2  | 1:162:A:THR:HB   | 6                   | 0.3      | 0.14                | 0.23       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 6                   | 0.3      | 0.13                | 0.26       |
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD3  | 6                   | 0.3      | 0.13                | 0.26       |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 6                   | 0.3      | 0.13                | 0.26       |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD3  | 6                   | 0.3      | 0.13                | 0.26       |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG21 | 6                   | 0.29     | 0.02                | 0.3        |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG22 | 6                   | 0.29     | 0.02                | 0.3        |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG23 | 6                   | 0.29     | 0.02                | 0.3        |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD11 | 6                   | 0.29     | 0.03                | 0.3        |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD12 | 6                   | 0.29     | 0.03                | 0.3        |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD13 | 6                   | 0.29     | 0.03                | 0.3        |
| (1,3748) | 1:113:B:THR:H    | 1:112:B:LYS:HB2  | 6                   | 0.29     | 0.08                | 0.28       |
| (1,3139) | 1:141:B:LYS:HG3  | 1:141:B:LYS:HE2  | 6                   | 0.29     | 0.05                | 0.3        |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE3  | 6                   | 0.28     | 0.08                | 0.29       |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE2  | 6                   | 0.28     | 0.08                | 0.29       |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE3  | 6                   | 0.28     | 0.14                | 0.26       |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE3  | 6                   | 0.28     | 0.14                | 0.26       |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE3  | 6                   | 0.28     | 0.14                | 0.26       |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE2  | 6                   | 0.28     | 0.14                | 0.26       |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE2  | 6                   | 0.28     | 0.14                | 0.26       |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE2  | 6                   | 0.28     | 0.14                | 0.26       |
| (1,4262) | 1:167:B:ALA:H    | 1:166:B:GLU:HB2  | 6                   | 0.28     | 0.14                | 0.26       |
| (1,1197) | 1:158:A:SER:HB3  | 1:159:A:PRO:HD3  | 6                   | 0.26     | 0.1                 | 0.24       |
| (1,1634) | 1:131:A:HIS:H    | 1:129:A:ASP:HB3  | 6                   | 0.24     | 0.06                | 0.22       |
| (1,3018) | 1:127:B:ARG:HA   | 1:127:B:ARG:HD3  | 6                   | 0.24     | 0.07                | 0.25       |
| (1,2738) | 1:112:B:LYS:HB2  | 1:120:B:ILE:HA   | 6                   | 0.23     | 0.08                | 0.22       |
| (1,3915) | 1:131:B:HIS:H    | 1:129:B:ASP:HB3  | 6                   | 0.22     | 0.09                | 0.22       |
| (1,4128) | 1:155:B:SER:H    | 1:154:B:SER:HB2  | 6                   | 0.22     | 0.08                | 0.22       |
| (1,2929) | 1:120:B:ILE:HG21 | 1:139:B:THR:HA   | 6                   | 0.22     | 0.06                | 0.22       |
| (1,2929) | 1:120:B:ILE:HG22 | 1:139:B:THR:HA   | 6                   | 0.22     | 0.06                | 0.22       |
| (1,2929) | 1:120:B:ILE:HG23 | 1:139:B:THR:HA   | 6                   | 0.22     | 0.06                | 0.22       |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD1  | 6                   | 0.21     | 0.07                | 0.22       |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD2  | 6                   | 0.21     | 0.07                | 0.22       |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD1  | 6                   | 0.21     | 0.07                | 0.22       |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD2  | 6                   | 0.21     | 0.07                | 0.22       |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD1  | 6                   | 0.21     | 0.07                | 0.22       |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD2  | 6                   | 0.21     | 0.07                | 0.22       |
| (1,2083) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 6                   | 0.2      | 0.05                | 0.22       |
| (1,2215) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 6                   | 0.2      | 0.05                | 0.22       |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG21 | 6                   | 0.2      | 0.06                | 0.19       |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG22 | 6                   | 0.2      | 0.06                | 0.19       |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG23 | 6                   | 0.2      | 0.06                | 0.19       |
| (1,1173) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB3  | 6                   | 0.2      | 0.04                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1173) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB3  | 6                   | 0.2      | 0.04                | 0.2        |
| (1,1173) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB3  | 6                   | 0.2      | 0.04                | 0.2        |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD21 | 6                   | 0.19     | 0.06                | 0.2        |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD22 | 6                   | 0.19     | 0.06                | 0.2        |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD23 | 6                   | 0.19     | 0.06                | 0.2        |
| (1,2928) | 1:120:B:ILE:HG21 | 1:122:B:GLY:HA3  | 6                   | 0.19     | 0.05                | 0.18       |
| (1,2928) | 1:120:B:ILE:HG22 | 1:122:B:GLY:HA3  | 6                   | 0.19     | 0.05                | 0.18       |
| (1,2928) | 1:120:B:ILE:HG23 | 1:122:B:GLY:HA3  | 6                   | 0.19     | 0.05                | 0.18       |
| (1,654)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD2  | 6                   | 0.18     | 0.09                | 0.15       |
| (1,654)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD2  | 6                   | 0.18     | 0.09                | 0.15       |
| (1,654)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD2  | 6                   | 0.18     | 0.09                | 0.15       |
| (1,279)  | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA2  | 6                   | 0.18     | 0.03                | 0.18       |
| (1,3358) | 1:153:B:VAL:HA   | 1:168:B:PRO:HD2  | 6                   | 0.18     | 0.03                | 0.18       |
| (1,652)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HB2  | 6                   | 0.17     | 0.09                | 0.14       |
| (1,652)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HB2  | 6                   | 0.17     | 0.09                | 0.14       |
| (1,652)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HB2  | 6                   | 0.17     | 0.09                | 0.14       |
| (1,1647) | 1:132:A:GLY:H    | 1:131:A:HIS:HB3  | 6                   | 0.17     | 0.03                | 0.18       |
| (1,4263) | 1:167:B:ALA:H    | 1:166:B:GLU:HB3  | 6                   | 0.17     | 0.06                | 0.16       |
| (1,664)  | 1:121:A:THR:HA   | 1:139:A:THR:HA   | 6                   | 0.17     | 0.04                | 0.16       |
| (1,1391) | 1:105:A:ALA:H    | 1:108:A:GLU:HB3  | 6                   | 0.16     | 0.03                | 0.18       |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG21 | 6                   | 0.15     | 0.04                | 0.15       |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG22 | 6                   | 0.15     | 0.04                | 0.15       |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG23 | 6                   | 0.15     | 0.04                | 0.15       |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD11 | 6                   | 0.14     | 0.04                | 0.12       |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD12 | 6                   | 0.14     | 0.04                | 0.12       |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD13 | 6                   | 0.14     | 0.04                | 0.12       |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG21 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG22 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG23 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,1079) | 1:153:A:VAL:HB   | 1:154:A:SER:HA   | 6                   | 0.13     | 0.02                | 0.12       |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG21 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG22 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG23 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,3928) | 1:132:B:GLY:H    | 1:131:B:HIS:HB3  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,141)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD1  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,141)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,141)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD1  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,141)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,141)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD1  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,141)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1311) | 1:170:A:PRO:HB2  | 1:170:A:PRO:HG2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,3592) | 1:170:B:PRO:HB2  | 1:170:B:PRO:HG2  | 6                   | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1301) | 1:169:A:MET:HB3  | 1:171:A:LYS:HG2  | 5                   | 1.25     | 0.28                | 1.13       |
| (1,1301) | 1:169:A:MET:HB3  | 1:171:A:LYS:HG3  | 5                   | 1.25     | 0.28                | 1.13       |
| (1,2004) | 1:171:A:LYS:H    | 1:169:A:MET:HA   | 5                   | 1.01     | 0.29                | 0.87       |
| (1,3346) | 1:152:B:GLN:HB2  | 1:169:B:MET:HA   | 5                   | 0.71     | 0.27                | 0.77       |
| (1,7)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HA    | 5                   | 0.65     | 0.26                | 0.63       |
| (1,1691) | 1:140:A:ARG:H    | 1:120:A:ILE:HB   | 5                   | 0.64     | 0.09                | 0.65       |
| (1,2062) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 5                   | 0.63     | 0.34                | 0.49       |
| (1,2194) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 5                   | 0.63     | 0.34                | 0.49       |
| (1,4255) | 1:167:B:ALA:H    | 1:95:B:TRP:HB3   | 5                   | 0.63     | 0.22                | 0.63       |
| (1,3763) | 1:114:B:LYS:H    | 1:115:B:ASP:HB2  | 5                   | 0.61     | 0.23                | 0.64       |
| (1,626)  | 1:120:A:ILE:HA   | 1:120:A:ILE:HG13 | 5                   | 0.56     | 0.02                | 0.55       |
| (1,4095) | 1:152:B:GLN:HE22 | 1:170:B:PRO:HD3  | 5                   | 0.52     | 0.16                | 0.5        |
| (1,232)  | 1:99:A:LEU:HD11  | 1:120:A:ILE:HG12 | 5                   | 0.52     | 0.16                | 0.59       |
| (1,232)  | 1:99:A:LEU:HD12  | 1:120:A:ILE:HG12 | 5                   | 0.52     | 0.16                | 0.59       |
| (1,232)  | 1:99:A:LEU:HD13  | 1:120:A:ILE:HG12 | 5                   | 0.52     | 0.16                | 0.59       |
| (1,2314) | 1:94:B:ARG:HA    | 1:169:B:MET:HB2  | 5                   | 0.51     | 0.12                | 0.45       |
| (1,3005) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB3  | 5                   | 0.5      | 0.47                | 0.22       |
| (1,3274) | 1:148:B:VAL:HA   | 1:170:B:PRO:HG2  | 5                   | 0.46     | 0.27                | 0.48       |
| (1,1799) | 1:152:A:GLN:HE21 | 1:152:A:GLN:HB3  | 5                   | 0.45     | 0.2                 | 0.43       |
| (1,4280) | 1:169:B:MET:H    | 1:169:B:MET:HB3  | 5                   | 0.45     | 0.23                | 0.45       |
| (1,682)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HE3  | 5                   | 0.42     | 0.16                | 0.44       |
| (1,682)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HE2  | 5                   | 0.42     | 0.16                | 0.44       |
| (1,449)  | 1:112:A:LYS:HA   | 1:112:A:LYS:HE2  | 5                   | 0.4      | 0.14                | 0.47       |
| (1,449)  | 1:112:A:LYS:HA   | 1:112:A:LYS:HE3  | 5                   | 0.4      | 0.14                | 0.47       |
| (1,2000) | 1:169:A:MET:H    | 1:169:A:MET:HG3  | 5                   | 0.4      | 0.23                | 0.5        |
| (1,3345) | 1:152:B:GLN:HB2  | 1:168:B:PRO:HD3  | 5                   | 0.4      | 0.23                | 0.38       |
| (1,528)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HB   | 5                   | 0.36     | 0.08                | 0.33       |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD1  | 5                   | 0.33     | 0.04                | 0.33       |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD2  | 5                   | 0.33     | 0.04                | 0.33       |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD1  | 5                   | 0.33     | 0.04                | 0.33       |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD2  | 5                   | 0.33     | 0.04                | 0.33       |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD1  | 5                   | 0.33     | 0.04                | 0.33       |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD2  | 5                   | 0.33     | 0.04                | 0.33       |
| (1,3902) | 1:129:B:ASP:H    | 1:129:B:ASP:HB2  | 5                   | 0.32     | 0.06                | 0.34       |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD11 | 5                   | 0.32     | 0.12                | 0.26       |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD12 | 5                   | 0.32     | 0.12                | 0.26       |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD13 | 5                   | 0.32     | 0.12                | 0.26       |
| (1,4205) | 1:162:B:THR:H    | 1:160:B:GLU:HB2  | 5                   | 0.31     | 0.08                | 0.31       |
| (1,3848) | 1:123:B:LYS:H    | 1:109:B:LEU:HG   | 5                   | 0.3      | 0.13                | 0.24       |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE1  | 5                   | 0.29     | 0.1                 | 0.28       |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE2  | 5                   | 0.29     | 0.1                 | 0.28       |
| (1,2993) | 1:126:B:GLU:HB3  | 1:133:B:TYR:HB2  | 5                   | 0.29     | 0.18                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2993) | 1:126:B:GLU:HB2  | 1:133:B:TYR:HB2  | 5                   | 0.29     | 0.18                | 0.16       |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG21 | 5                   | 0.27     | 0.03                | 0.27       |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG22 | 5                   | 0.27     | 0.03                | 0.27       |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG23 | 5                   | 0.27     | 0.03                | 0.27       |
| (1,1847) | 1:155:A:SER:H    | 1:154:A:SER:HB2  | 5                   | 0.27     | 0.07                | 0.29       |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD11 | 5                   | 0.27     | 0.15                | 0.21       |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD12 | 5                   | 0.27     | 0.15                | 0.21       |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD13 | 5                   | 0.27     | 0.15                | 0.21       |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD11 | 5                   | 0.25     | 0.07                | 0.27       |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD12 | 5                   | 0.25     | 0.07                | 0.27       |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD13 | 5                   | 0.25     | 0.07                | 0.27       |
| (1,1816) | 1:153:A:VAL:H    | 1:149:A:ASP:HB2  | 5                   | 0.24     | 0.11                | 0.21       |
| (1,1065) | 1:152:A:GLN:HB2  | 1:169:A:MET:HA   | 5                   | 0.24     | 0.07                | 0.24       |
| (1,858)  | 1:141:A:LYS:HG3  | 1:141:A:LYS:HE2  | 5                   | 0.22     | 0.07                | 0.2        |
| (1,1626) | 1:129:A:ASP:H    | 1:132:A:GLY:HA3  | 5                   | 0.22     | 0.04                | 0.23       |
| (1,1280) | 1:168:A:PRO:HB2  | 1:170:A:PRO:HD3  | 5                   | 0.22     | 0.1                 | 0.24       |
| (1,3249) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA3  | 5                   | 0.22     | 0.18                | 0.13       |
| (1,3474) | 1:158:B:SER:HB3  | 1:160:B:GLU:HB3  | 5                   | 0.22     | 0.12                | 0.13       |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD1  | 5                   | 0.21     | 0.12                | 0.15       |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD2  | 5                   | 0.21     | 0.12                | 0.15       |
| (1,1703) | 1:142:A:TYR:H    | 1:141:A:LYS:HG3  | 5                   | 0.21     | 0.06                | 0.22       |
| (1,1703) | 1:142:A:TYR:H    | 1:141:A:LYS:HG2  | 5                   | 0.21     | 0.06                | 0.22       |
| (1,80)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HD2   | 5                   | 0.21     | 0.06                | 0.23       |
| (1,80)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HD3   | 5                   | 0.21     | 0.06                | 0.23       |
| (1,3910) | 1:129:B:ASP:H    | 1:133:B:TYR:HB2  | 5                   | 0.21     | 0.1                 | 0.17       |
| (1,3955) | 1:137:B:CYS:H    | 1:136:B:ARG:HB3  | 5                   | 0.21     | 0.07                | 0.22       |
| (1,4182) | 1:161:B:GLY:H    | 1:102:B:ASN:HB2  | 5                   | 0.2      | 0.08                | 0.2        |
| (1,1598) | 1:128:A:GLN:H    | 1:127:A:ARG:HG2  | 5                   | 0.2      | 0.08                | 0.22       |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD21 | 5                   | 0.2      | 0.08                | 0.16       |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD22 | 5                   | 0.2      | 0.08                | 0.16       |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD23 | 5                   | 0.2      | 0.08                | 0.16       |
| (1,3454) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB3  | 5                   | 0.19     | 0.05                | 0.17       |
| (1,3454) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB3  | 5                   | 0.19     | 0.05                | 0.17       |
| (1,3454) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB3  | 5                   | 0.19     | 0.05                | 0.17       |
| (1,1580) | 1:125:A:GLU:H    | 1:108:A:GLU:HG2  | 5                   | 0.18     | 0.07                | 0.21       |
| (1,364)  | 1:109:A:LEU:HG   | 1:120:A:ILE:HD11 | 5                   | 0.18     | 0.05                | 0.18       |
| (1,364)  | 1:109:A:LEU:HG   | 1:120:A:ILE:HD12 | 5                   | 0.18     | 0.05                | 0.18       |
| (1,364)  | 1:109:A:LEU:HG   | 1:120:A:ILE:HD13 | 5                   | 0.18     | 0.05                | 0.18       |
| (1,2977) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB3  | 5                   | 0.18     | 0.09                | 0.11       |
| (1,2977) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HB3  | 5                   | 0.18     | 0.09                | 0.11       |
| (1,1525) | 1:119:A:GLU:H    | 1:114:A:LYS:HB3  | 5                   | 0.17     | 0.05                | 0.17       |
| (1,3430) | 1:157:B:LEU:HA   | 1:163:B:LEU:HB3  | 5                   | 0.17     | 0.02                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG21 | 5                   | 0.17     | 0.02                | 0.17       |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG22 | 5                   | 0.17     | 0.02                | 0.17       |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG23 | 5                   | 0.17     | 0.02                | 0.17       |
| (1,782)  | 1:131:A:HIS:HB2  | 1:132:A:GLY:HA2  | 5                   | 0.16     | 0.06                | 0.13       |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG21 | 5                   | 0.16     | 0.04                | 0.14       |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG22 | 5                   | 0.16     | 0.04                | 0.14       |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG23 | 5                   | 0.16     | 0.04                | 0.14       |
| (1,1901) | 1:161:A:GLY:H    | 1:102:A:ASN:HB2  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG21 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG22 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG23 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG21 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG22 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG23 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG21 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG22 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG23 | 5                   | 0.16     | 0.05                | 0.13       |
| (1,605)  | 1:119:A:GLU:HA   | 1:120:A:ILE:HG13 | 5                   | 0.15     | 0.01                | 0.16       |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD21 | 5                   | 0.15     | 0.03                | 0.16       |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD22 | 5                   | 0.15     | 0.03                | 0.16       |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD23 | 5                   | 0.15     | 0.03                | 0.16       |
| (1,1282) | 1:168:A:PRO:HB3  | 1:169:A:MET:HA   | 5                   | 0.15     | 0.04                | 0.14       |
| (1,3391) | 1:155:B:SER:HA   | 1:165:B:VAL:HA   | 5                   | 0.15     | 0.03                | 0.15       |
| (1,546)  | 1:117:A:VAL:HA   | 1:143:A:THR:HG21 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,546)  | 1:117:A:VAL:HA   | 1:143:A:THR:HG22 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,546)  | 1:117:A:VAL:HA   | 1:143:A:THR:HG23 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE1  | 5                   | 0.14     | 0.04                | 0.13       |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE2  | 5                   | 0.14     | 0.04                | 0.13       |
| (1,857)  | 1:141:A:LYS:HG2  | 1:143:A:THR:HA   | 5                   | 0.14     | 0.03                | 0.14       |
| (1,1588) | 1:126:A:GLU:H    | 1:125:A:GLU:HG3  | 5                   | 0.14     | 0.02                | 0.13       |
| (1,2442) | 1:97:B:VAL:HG21  | 1:166:B:GLU:HA   | 5                   | 0.14     | 0.03                | 0.12       |
| (1,2442) | 1:97:B:VAL:HG22  | 1:166:B:GLU:HA   | 5                   | 0.14     | 0.03                | 0.12       |
| (1,2442) | 1:97:B:VAL:HG23  | 1:166:B:GLU:HA   | 5                   | 0.14     | 0.03                | 0.12       |
| (1,1110) | 1:155:A:SER:HA   | 1:165:A:VAL:HA   | 5                   | 0.14     | 0.01                | 0.14       |
| (1,2831) | 1:117:B:VAL:HA   | 1:148:B:VAL:HB   | 5                   | 0.14     | 0.03                | 0.15       |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG21 | 5                   | 0.14     | 0.03                | 0.13       |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG22 | 5                   | 0.14     | 0.03                | 0.13       |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG23 | 5                   | 0.14     | 0.03                | 0.13       |
| (1,3015) | 1:127:B:ARG:HA   | 1:127:B:ARG:HB3  | 5                   | 0.14     | 0.04                | 0.13       |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG21 | 5                   | 0.13     | 0.02                | 0.14       |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG22 | 5                   | 0.13     | 0.02                | 0.14       |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG23 | 5                   | 0.13     | 0.02                | 0.14       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD21 | 5                   | 0.12     | 0.02                | 0.12       |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD22 | 5                   | 0.12     | 0.02                | 0.12       |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD23 | 5                   | 0.12     | 0.02                | 0.12       |
| (1,734)  | 1:127:A:ARG:HA   | 1:127:A:ARG:HB3  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD11 | 5                   | 0.12     | 0.01                | 0.11       |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD12 | 5                   | 0.12     | 0.01                | 0.11       |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD13 | 5                   | 0.12     | 0.01                | 0.11       |
| (1,724)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB3  | 4                   | 0.95     | 0.32                | 1.06       |
| (1,16)   | 1:93:A:ASP:HA    | 1:94:A:ARG:HD2   | 4                   | 0.86     | 0.4                 | 0.8        |
| (1,4076) | 1:152:B:GLN:H    | 1:170:B:PRO:HD2  | 4                   | 0.7      | 0.32                | 0.79       |
| (1,4076) | 1:152:B:GLN:H    | 1:170:B:PRO:HD3  | 4                   | 0.7      | 0.32                | 0.79       |
| (1,728)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HA   | 4                   | 0.62     | 0.21                | 0.64       |
| (1,2009) | 1:171:A:LYS:H    | 1:171:A:LYS:HB2  | 4                   | 0.6      | 0.26                | 0.6        |
| (1,2009) | 1:171:A:LYS:H    | 1:171:A:LYS:HB3  | 4                   | 0.6      | 0.26                | 0.6        |
| (1,2007) | 1:171:A:LYS:H    | 1:170:A:PRO:HD3  | 4                   | 0.55     | 0.21                | 0.59       |
| (1,3895) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB2  | 4                   | 0.55     | 0.14                | 0.5        |
| (1,3126) | 1:141:B:LYS:HA   | 1:141:B:LYS:HD3  | 4                   | 0.52     | 0.07                | 0.56       |
| (1,3126) | 1:141:B:LYS:HA   | 1:141:B:LYS:HD2  | 4                   | 0.52     | 0.07                | 0.56       |
| (1,1288) | 1:169:A:MET:HA   | 1:169:A:MET:HG2  | 4                   | 0.52     | 0.11                | 0.52       |
| (1,4024) | 1:148:B:VAL:H    | 1:146:B:PRO:HB3  | 4                   | 0.5      | 0.1                 | 0.53       |
| (1,1322) | 1:94:A:ARG:H     | 1:93:A:ASP:HB2   | 4                   | 0.48     | 0.11                | 0.48       |
| (1,2318) | 1:94:B:ARG:HB2   | 1:96:B:ARG:HA    | 4                   | 0.47     | 0.33                | 0.36       |
| (1,3972) | 1:140:B:ARG:H    | 1:120:B:ILE:HB   | 4                   | 0.47     | 0.12                | 0.5        |
| (1,255)  | 1:99:A:LEU:HD21  | 1:109:A:LEU:HG   | 4                   | 0.46     | 0.13                | 0.52       |
| (1,255)  | 1:99:A:LEU:HD22  | 1:109:A:LEU:HG   | 4                   | 0.46     | 0.13                | 0.52       |
| (1,255)  | 1:99:A:LEU:HD23  | 1:109:A:LEU:HG   | 4                   | 0.46     | 0.13                | 0.52       |
| (1,3116) | 1:139:B:THR:HG21 | 1:141:B:LYS:HE2  | 4                   | 0.45     | 0.14                | 0.49       |
| (1,3116) | 1:139:B:THR:HG22 | 1:141:B:LYS:HE2  | 4                   | 0.45     | 0.14                | 0.49       |
| (1,3116) | 1:139:B:THR:HG23 | 1:141:B:LYS:HE2  | 4                   | 0.45     | 0.14                | 0.49       |
| (1,1114) | 1:155:A:SER:HB2  | 1:163:A:LEU:HA   | 4                   | 0.45     | 0.16                | 0.48       |
| (1,4025) | 1:148:B:VAL:H    | 1:146:B:PRO:HG2  | 4                   | 0.45     | 0.12                | 0.48       |
| (1,2148) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 4                   | 0.44     | 0.23                | 0.38       |
| (1,2281) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 4                   | 0.44     | 0.23                | 0.38       |
| (1,2980) | 1:125:B:GLU:HA   | 1:125:B:GLU:HG2  | 4                   | 0.42     | 0.15                | 0.5        |
| (1,2299) | 1:93:B:ASP:HB2   | 1:94:B:ARG:HA    | 4                   | 0.4      | 0.08                | 0.37       |
| (1,3569) | 1:169:B:MET:HA   | 1:169:B:MET:HG2  | 4                   | 0.4      | 0.23                | 0.4        |
| (1,455)  | 1:112:A:LYS:HB2  | 1:112:A:LYS:HE2  | 4                   | 0.39     | 0.07                | 0.42       |
| (1,455)  | 1:112:A:LYS:HB2  | 1:112:A:LYS:HE3  | 4                   | 0.39     | 0.07                | 0.42       |
| (1,405)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HD2  | 4                   | 0.38     | 0.22                | 0.34       |
| (1,405)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HD2  | 4                   | 0.38     | 0.22                | 0.34       |
| (1,405)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HD2  | 4                   | 0.38     | 0.22                | 0.34       |
| (1,405)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HD3  | 4                   | 0.38     | 0.22                | 0.34       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,405)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HD3  | 4                   | 0.38     | 0.22                | 0.34       |
| (1,405)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HD3  | 4                   | 0.38     | 0.22                | 0.34       |
| (1,2930) | 1:120:B:ILE:HG21 | 1:140:B:ARG:HA   | 4                   | 0.38     | 0.14                | 0.36       |
| (1,2930) | 1:120:B:ILE:HG22 | 1:140:B:ARG:HA   | 4                   | 0.38     | 0.14                | 0.36       |
| (1,2930) | 1:120:B:ILE:HG23 | 1:140:B:ARG:HA   | 4                   | 0.38     | 0.14                | 0.36       |
| (1,1277) | 1:168:A:PRO:HA   | 1:169:A:MET:HG3  | 4                   | 0.38     | 0.24                | 0.38       |
| (1,4084) | 1:152:B:GLN:HE21 | 1:168:B:PRO:HD2  | 4                   | 0.38     | 0.13                | 0.39       |
| (1,434)  | 1:111:A:VAL:HG11 | 1:120:A:ILE:HG12 | 4                   | 0.37     | 0.08                | 0.39       |
| (1,434)  | 1:111:A:VAL:HG12 | 1:120:A:ILE:HG12 | 4                   | 0.37     | 0.08                | 0.39       |
| (1,434)  | 1:111:A:VAL:HG13 | 1:120:A:ILE:HG12 | 4                   | 0.37     | 0.08                | 0.39       |
| (1,1756) | 1:148:A:VAL:H    | 1:170:A:PRO:HG3  | 4                   | 0.36     | 0.13                | 0.36       |
| (1,845)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HD3  | 4                   | 0.36     | 0.17                | 0.34       |
| (1,845)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HD2  | 4                   | 0.36     | 0.17                | 0.34       |
| (1,1664) | 1:135:A:SER:H    | 1:134:A:ILE:HG13 | 4                   | 0.36     | 0.11                | 0.38       |
| (1,2971) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HB2  | 4                   | 0.35     | 0.12                | 0.34       |
| (1,690)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HB2  | 4                   | 0.34     | 0.13                | 0.38       |
| (1,3604) | 1:94:B:ARG:H     | 1:93:B:ASP:HB3   | 4                   | 0.32     | 0.11                | 0.29       |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD21 | 4                   | 0.31     | 0.14                | 0.32       |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD22 | 4                   | 0.31     | 0.14                | 0.32       |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD23 | 4                   | 0.31     | 0.14                | 0.32       |
| (1,712)  | 1:126:A:GLU:HB3  | 1:133:A:TYR:HB2  | 4                   | 0.29     | 0.18                | 0.28       |
| (1,1642) | 1:132:A:GLY:H    | 1:129:A:ASP:HB2  | 4                   | 0.29     | 0.16                | 0.26       |
| (1,166)  | 1:97:A:VAL:HG21  | 1:118:A:VAL:HB   | 4                   | 0.29     | 0.07                | 0.3        |
| (1,166)  | 1:97:A:VAL:HG22  | 1:118:A:VAL:HB   | 4                   | 0.29     | 0.07                | 0.3        |
| (1,166)  | 1:97:A:VAL:HG23  | 1:118:A:VAL:HB   | 4                   | 0.29     | 0.07                | 0.3        |
| (1,166)  | 1:97:A:VAL:HG11  | 1:118:A:VAL:HB   | 4                   | 0.29     | 0.07                | 0.3        |
| (1,166)  | 1:97:A:VAL:HG12  | 1:118:A:VAL:HB   | 4                   | 0.29     | 0.07                | 0.3        |
| (1,166)  | 1:97:A:VAL:HG13  | 1:118:A:VAL:HB   | 4                   | 0.29     | 0.07                | 0.3        |
| (1,2963) | 1:123:B:LYS:HA   | 1:123:B:LYS:HE3  | 4                   | 0.28     | 0.16                | 0.28       |
| (1,2963) | 1:123:B:LYS:HA   | 1:123:B:LYS:HE2  | 4                   | 0.28     | 0.16                | 0.28       |
| (1,2753) | 1:112:B:LYS:HD3  | 1:120:B:ILE:HA   | 4                   | 0.27     | 0.15                | 0.24       |
| (1,2753) | 1:112:B:LYS:HD2  | 1:120:B:ILE:HA   | 4                   | 0.27     | 0.15                | 0.24       |
| (1,2332) | 1:95:B:TRP:HA    | 1:95:B:TRP:HB2   | 4                   | 0.27     | 0.08                | 0.25       |
| (1,2568) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB3  | 4                   | 0.27     | 0.1                 | 0.29       |
| (1,2617) | 1:108:B:GLU:HA   | 1:108:B:GLU:HG2  | 4                   | 0.26     | 0.1                 | 0.28       |
| (1,2935) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HD2  | 4                   | 0.26     | 0.1                 | 0.26       |
| (1,2935) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HD2  | 4                   | 0.26     | 0.1                 | 0.26       |
| (1,2935) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HD2  | 4                   | 0.26     | 0.1                 | 0.26       |
| (1,3935) | 1:134:B:ILE:H    | 1:127:B:ARG:HB2  | 4                   | 0.26     | 0.08                | 0.29       |
| (1,3302) | 1:148:B:VAL:HG21 | 1:169:B:MET:HB3  | 4                   | 0.25     | 0.06                | 0.25       |
| (1,3302) | 1:148:B:VAL:HG22 | 1:169:B:MET:HB3  | 4                   | 0.25     | 0.06                | 0.25       |
| (1,3302) | 1:148:B:VAL:HG23 | 1:169:B:MET:HB3  | 4                   | 0.25     | 0.06                | 0.25       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,457)  | 1:112:A:LYS:HB2  | 1:120:A:ILE:HA   | 4                   | 0.24     | 0.06                | 0.22       |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD21 | 4                   | 0.24     | 0.06                | 0.22       |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD22 | 4                   | 0.24     | 0.06                | 0.22       |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD23 | 4                   | 0.24     | 0.06                | 0.22       |
| (1,1314) | 1:170:A:PRO:HB3  | 1:170:A:PRO:HD3  | 4                   | 0.23     | 0.03                | 0.22       |
| (1,1314) | 1:170:A:PRO:HB3  | 1:170:A:PRO:HD2  | 4                   | 0.23     | 0.03                | 0.22       |
| (1,3806) | 1:119:B:GLU:H    | 1:114:B:LYS:HB3  | 4                   | 0.23     | 0.1                 | 0.2        |
| (1,650)  | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD1  | 4                   | 0.23     | 0.1                 | 0.23       |
| (1,650)  | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD2  | 4                   | 0.23     | 0.1                 | 0.23       |
| (1,650)  | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD1  | 4                   | 0.23     | 0.1                 | 0.23       |
| (1,650)  | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD2  | 4                   | 0.23     | 0.1                 | 0.23       |
| (1,650)  | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD1  | 4                   | 0.23     | 0.1                 | 0.23       |
| (1,650)  | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD2  | 4                   | 0.23     | 0.1                 | 0.23       |
| (1,3907) | 1:129:B:ASP:H    | 1:132:B:GLY:HA3  | 4                   | 0.23     | 0.07                | 0.21       |
| (1,262)  | 1:100:A:ASP:HA   | 1:162:A:THR:HG21 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,262)  | 1:100:A:ASP:HA   | 1:162:A:THR:HG22 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,262)  | 1:100:A:ASP:HA   | 1:162:A:THR:HG23 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,1743) | 1:148:A:VAL:H    | 1:146:A:PRO:HB3  | 4                   | 0.22     | 0.15                | 0.15       |
| (1,3138) | 1:141:B:LYS:HG2  | 1:143:B:THR:HA   | 4                   | 0.22     | 0.04                | 0.22       |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG21  | 4                   | 0.22     | 0.1                 | 0.18       |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG22  | 4                   | 0.22     | 0.1                 | 0.18       |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG23  | 4                   | 0.22     | 0.1                 | 0.18       |
| (1,1902) | 1:161:A:GLY:H    | 1:102:A:ASN:HB3  | 4                   | 0.21     | 0.06                | 0.2        |
| (1,831)  | 1:139:A:THR:HB   | 1:141:A:LYS:HE2  | 4                   | 0.21     | 0.06                | 0.21       |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD11 | 4                   | 0.21     | 0.05                | 0.23       |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD12 | 4                   | 0.21     | 0.05                | 0.23       |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD13 | 4                   | 0.21     | 0.05                | 0.23       |
| (1,648)  | 1:120:A:ILE:HG21 | 1:139:A:THR:HA   | 4                   | 0.2      | 0.08                | 0.2        |
| (1,648)  | 1:120:A:ILE:HG22 | 1:139:A:THR:HA   | 4                   | 0.2      | 0.08                | 0.2        |
| (1,648)  | 1:120:A:ILE:HG23 | 1:139:A:THR:HA   | 4                   | 0.2      | 0.08                | 0.2        |
| (1,1796) | 1:152:A:GLN:HE21 | 1:149:A:ASP:HB2  | 4                   | 0.2      | 0.04                | 0.22       |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD1  | 4                   | 0.2      | 0.06                | 0.22       |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD2  | 4                   | 0.2      | 0.06                | 0.22       |
| (1,337)  | 1:108:A:GLU:HA   | 1:108:A:GLU:HG3  | 4                   | 0.2      | 0.04                | 0.18       |
| (1,2560) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA2  | 4                   | 0.19     | 0.03                | 0.2        |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG11 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG12 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG13 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG11 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG12 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG13 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG11 | 4                   | 0.19     | 0.06                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG12 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG13 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,2945) | 1:121:B:THR:HA   | 1:139:B:THR:HA   | 4                   | 0.19     | 0.03                | 0.19       |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG11 | 4                   | 0.18     | 0.07                | 0.17       |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG12 | 4                   | 0.18     | 0.07                | 0.17       |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG13 | 4                   | 0.18     | 0.07                | 0.17       |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG11 | 4                   | 0.18     | 0.07                | 0.17       |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG12 | 4                   | 0.18     | 0.07                | 0.17       |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG13 | 4                   | 0.18     | 0.07                | 0.17       |
| (1,2329) | 1:94:B:ARG:HD2   | 1:168:B:PRO:HA   | 4                   | 0.18     | 0.08                | 0.16       |
| (1,1655) | 1:134:A:ILE:H    | 1:127:A:ARG:HG2  | 4                   | 0.18     | 0.04                | 0.18       |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG21 | 4                   | 0.18     | 0.05                | 0.16       |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG22 | 4                   | 0.18     | 0.05                | 0.16       |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG23 | 4                   | 0.18     | 0.05                | 0.16       |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG21 | 4                   | 0.18     | 0.02                | 0.17       |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG22 | 4                   | 0.18     | 0.02                | 0.17       |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG23 | 4                   | 0.18     | 0.02                | 0.17       |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD11 | 4                   | 0.17     | 0.06                | 0.16       |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD12 | 4                   | 0.17     | 0.06                | 0.16       |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD13 | 4                   | 0.17     | 0.06                | 0.16       |
| (1,3143) | 1:141:B:LYS:HG3  | 1:142:B:TYR:HB3  | 4                   | 0.16     | 0.03                | 0.17       |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG21 | 4                   | 0.16     | 0.03                | 0.18       |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG22 | 4                   | 0.16     | 0.03                | 0.18       |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG23 | 4                   | 0.16     | 0.03                | 0.18       |
| (1,4089) | 1:152:B:GLN:HE22 | 1:152:B:GLN:HB2  | 4                   | 0.16     | 0.03                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG21 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG22 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG23 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG21 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG22 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG23 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG21 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG22 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,432)  | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG23 | 4                   | 0.16     | 0.04                | 0.16       |
| (1,419)  | 1:111:A:VAL:HA   | 1:120:A:ILE:HG13 | 4                   | 0.16     | 0.03                | 0.16       |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG21 | 4                   | 0.16     | 0.01                | 0.16       |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG22 | 4                   | 0.16     | 0.01                | 0.16       |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG23 | 4                   | 0.16     | 0.01                | 0.16       |
| (1,562)  | 1:117:A:VAL:HG11 | 1:142:A:TYR:HB3  | 4                   | 0.15     | 0.04                | 0.16       |
| (1,562)  | 1:117:A:VAL:HG12 | 1:142:A:TYR:HB3  | 4                   | 0.15     | 0.04                | 0.16       |
| (1,562)  | 1:117:A:VAL:HG13 | 1:142:A:TYR:HB3  | 4                   | 0.15     | 0.04                | 0.16       |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB1  | 4                   | 0.15     | 0.06                | 0.13       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB2  | 4                   | 0.15     | 0.06                | 0.13       |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB3  | 4                   | 0.15     | 0.06                | 0.13       |
| (1,2578) | 1:105:B:ALA:HB1  | 1:107:B:ASP:HB3  | 4                   | 0.15     | 0.05                | 0.14       |
| (1,2578) | 1:105:B:ALA:HB2  | 1:107:B:ASP:HB3  | 4                   | 0.15     | 0.05                | 0.14       |
| (1,2578) | 1:105:B:ALA:HB3  | 1:107:B:ASP:HB3  | 4                   | 0.15     | 0.05                | 0.14       |
| (1,2892) | 1:119:B:GLU:HA   | 1:141:B:LYS:HE2  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,361)  | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD21 | 4                   | 0.15     | 0.01                | 0.15       |
| (1,361)  | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD22 | 4                   | 0.15     | 0.01                | 0.15       |
| (1,361)  | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD23 | 4                   | 0.15     | 0.01                | 0.15       |
| (1,513)  | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG21 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,513)  | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG22 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,513)  | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG23 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD11 | 4                   | 0.15     | 0.01                | 0.15       |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD12 | 4                   | 0.15     | 0.01                | 0.15       |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD13 | 4                   | 0.15     | 0.01                | 0.15       |
| (1,1517) | 1:118:A:VAL:H    | 1:142:A:TYR:HB2  | 4                   | 0.14     | 0.04                | 0.14       |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD21 | 4                   | 0.14     | 0.03                | 0.14       |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD22 | 4                   | 0.14     | 0.03                | 0.14       |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD23 | 4                   | 0.14     | 0.03                | 0.14       |
| (1,4183) | 1:161:B:GLY:H    | 1:102:B:ASN:HB3  | 4                   | 0.14     | 0.04                | 0.13       |
| (1,2093) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2093) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2093) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2225) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2225) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2225) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,3360) | 1:153:B:VAL:HB   | 1:154:B:SER:HA   | 4                   | 0.14     | 0.01                | 0.14       |
| (1,3770) | 1:114:B:LYS:H    | 1:119:B:GLU:H    | 4                   | 0.14     | 0.02                | 0.15       |
| (1,3292) | 1:148:B:VAL:HG11 | 1:169:B:MET:HA   | 4                   | 0.14     | 0.02                | 0.14       |
| (1,3292) | 1:148:B:VAL:HG12 | 1:169:B:MET:HA   | 4                   | 0.14     | 0.02                | 0.14       |
| (1,3292) | 1:148:B:VAL:HG13 | 1:169:B:MET:HA   | 4                   | 0.14     | 0.02                | 0.14       |
| (1,3438) | 1:157:B:LEU:HB3  | 1:157:B:LEU:HG   | 4                   | 0.14     | 0.01                | 0.14       |
| (1,1172) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB2  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1172) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB2  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1172) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB2  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD11 | 4                   | 0.13     | 0.02                | 0.13       |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD12 | 4                   | 0.13     | 0.02                | 0.13       |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD13 | 4                   | 0.13     | 0.02                | 0.13       |
| (1,1345) | 1:97:A:VAL:H     | 1:165:A:VAL:H    | 4                   | 0.13     | 0.01                | 0.12       |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD11 | 4                   | 0.13     | 0.01                | 0.12       |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD12 | 4                   | 0.13     | 0.01                | 0.12       |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD13 | 4                   | 0.13     | 0.01                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2886) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG13 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD11 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD12 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD13 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1627) | 1:129:A:ASP:H    | 1:132:A:GLY:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,3670) | 1:105:B:ALA:H    | 1:106:B:PRO:HD3  | 4                   | 0.11     | 0.01                | 0.12       |
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG21 | 4                   | 0.11     | 0.01                | 0.12       |
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG22 | 4                   | 0.11     | 0.01                | 0.12       |
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG23 | 4                   | 0.11     | 0.01                | 0.12       |
| (1,2290) | 1:90:B:HIS:HB3   | 1:91:B:THR:HA    | 3                   | 0.93     | 0.31                | 0.83       |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE1  | 3                   | 0.82     | 0.51                | 0.58       |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE2  | 3                   | 0.82     | 0.51                | 0.58       |
| (1,3601) | 1:94:B:ARG:H     | 1:92:B:ALA:HA    | 3                   | 0.81     | 0.55                | 0.45       |
| (1,4285) | 1:171:B:LYS:H    | 1:169:B:MET:HA   | 3                   | 0.79     | 0.38                | 0.65       |
| (1,4293) | 1:172:B:LEU:H    | 1:171:B:LYS:HA   | 3                   | 0.73     | 0.26                | 0.85       |
| (1,4272) | 1:169:B:MET:H    | 1:95:B:TRP:HA    | 3                   | 0.67     | 0.16                | 0.76       |
| (1,4080) | 1:152:B:GLN:HE21 | 1:152:B:GLN:HB3  | 3                   | 0.65     | 0.09                | 0.61       |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB1  | 3                   | 0.6      | 0.31                | 0.4        |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB2  | 3                   | 0.6      | 0.31                | 0.4        |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB3  | 3                   | 0.6      | 0.31                | 0.4        |
| (1,3303) | 1:148:B:VAL:HG21 | 1:170:B:PRO:HG2  | 3                   | 0.59     | 0.22                | 0.46       |
| (1,3303) | 1:148:B:VAL:HG22 | 1:170:B:PRO:HG2  | 3                   | 0.59     | 0.22                | 0.46       |
| (1,3303) | 1:148:B:VAL:HG23 | 1:170:B:PRO:HG2  | 3                   | 0.59     | 0.22                | 0.46       |
| (1,2346) | 1:95:B:TRP:HB3   | 1:95:B:TRP:HE3   | 3                   | 0.56     | 0.03                | 0.57       |
| (1,65)   | 1:95:A:TRP:HB3   | 1:95:A:TRP:HE3   | 3                   | 0.56     | 0.01                | 0.56       |
| (1,4048) | 1:149:B:ASP:H    | 1:170:B:PRO:HG3  | 3                   | 0.53     | 0.2                 | 0.62       |
| (1,3603) | 1:94:B:ARG:H     | 1:93:B:ASP:HB2   | 3                   | 0.53     | 0.09                | 0.54       |
| (1,2513) | 1:99:B:LEU:HD11  | 1:120:B:ILE:HG12 | 3                   | 0.49     | 0.09                | 0.43       |
| (1,2513) | 1:99:B:LEU:HD12  | 1:120:B:ILE:HG12 | 3                   | 0.49     | 0.09                | 0.43       |
| (1,2513) | 1:99:B:LEU:HD13  | 1:120:B:ILE:HG12 | 3                   | 0.49     | 0.09                | 0.43       |
| (1,1623) | 1:129:A:ASP:H    | 1:130:A:GLU:HG3  | 3                   | 0.48     | 0.08                | 0.44       |
| (1,3557) | 1:168:B:PRO:HA   | 1:169:B:MET:HG2  | 3                   | 0.47     | 0.4                 | 0.23       |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG21  | 3                   | 0.47     | 0.26                | 0.42       |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG22  | 3                   | 0.47     | 0.26                | 0.42       |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG23  | 3                   | 0.47     | 0.26                | 0.42       |
| (1,1331) | 1:95:A:TRP:H     | 1:95:A:TRP:HB2   | 3                   | 0.46     | 0.04                | 0.47       |
| (1,406)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HE3  | 3                   | 0.45     | 0.13                | 0.39       |
| (1,406)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HE3  | 3                   | 0.45     | 0.13                | 0.39       |
| (1,406)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HE3  | 3                   | 0.45     | 0.13                | 0.39       |
| (1,715)  | 1:126:A:GLU:HB2  | 1:135:A:SER:HB3  | 3                   | 0.44     | 0.21                | 0.32       |
| (1,3613) | 1:95:B:TRP:H     | 1:95:B:TRP:HE3   | 3                   | 0.43     | 0.08                | 0.45       |
| (1,18)   | 1:93:A:ASP:HB2   | 1:94:A:ARG:HA    | 3                   | 0.42     | 0.12                | 0.5        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3096) | 1:136:B:ARG:HG3  | 1:138:B:PHE:HA   | 3                   | 0.42     | 0.19                | 0.32       |
| (1,1640) | 1:132:A:GLY:H    | 1:128:A:GLN:HG2  | 3                   | 0.41     | 0.07                | 0.44       |
| (1,1332) | 1:95:A:TRP:H     | 1:95:A:TRP:HE3   | 3                   | 0.4      | 0.03                | 0.41       |
| (1,3013) | 1:126:B:GLU:HG3  | 1:134:B:ILE:HG23 | 3                   | 0.39     | 0.21                | 0.42       |
| (1,3013) | 1:126:B:GLU:HG3  | 1:134:B:ILE:HG22 | 3                   | 0.39     | 0.21                | 0.42       |
| (1,805)  | 1:134:A:ILE:HD13 | 1:135:A:SER:HB2  | 3                   | 0.38     | 0.18                | 0.44       |
| (1,805)  | 1:134:A:ILE:HD11 | 1:135:A:SER:HB2  | 3                   | 0.38     | 0.18                | 0.44       |
| (1,805)  | 1:134:A:ILE:HG21 | 1:135:A:SER:HB2  | 3                   | 0.38     | 0.18                | 0.44       |
| (1,2715) | 1:111:B:VAL:HG11 | 1:120:B:ILE:HG12 | 3                   | 0.38     | 0.12                | 0.3        |
| (1,2715) | 1:111:B:VAL:HG12 | 1:120:B:ILE:HG12 | 3                   | 0.38     | 0.12                | 0.3        |
| (1,2715) | 1:111:B:VAL:HG13 | 1:120:B:ILE:HG12 | 3                   | 0.38     | 0.12                | 0.3        |
| (1,2619) | 1:108:B:GLU:HA   | 1:123:B:LYS:HD2  | 3                   | 0.37     | 0.22                | 0.27       |
| (1,2625) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HD2  | 3                   | 0.37     | 0.15                | 0.27       |
| (1,704)  | 1:125:A:GLU:HA   | 1:135:A:SER:HB3  | 3                   | 0.37     | 0.35                | 0.13       |
| (1,1974) | 1:167:A:ALA:H    | 1:95:A:TRP:HB3   | 3                   | 0.37     | 0.04                | 0.36       |
| (1,33)   | 1:94:A:ARG:HA    | 1:169:A:MET:HB2  | 3                   | 0.35     | 0.18                | 0.37       |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB1   | 3                   | 0.35     | 0.21                | 0.3        |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB2   | 3                   | 0.35     | 0.21                | 0.3        |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB3   | 3                   | 0.35     | 0.21                | 0.3        |
| (1,3092) | 1:136:B:ARG:HA   | 1:136:B:ARG:HG2  | 3                   | 0.35     | 0.06                | 0.38       |
| (1,1924) | 1:162:A:THR:H    | 1:160:A:GLU:HB2  | 3                   | 0.35     | 0.11                | 0.4        |
| (1,612)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HE3  | 3                   | 0.33     | 0.1                 | 0.33       |
| (1,2075) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 3                   | 0.33     | 0.08                | 0.28       |
| (1,2075) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 3                   | 0.33     | 0.08                | 0.28       |
| (1,2075) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 3                   | 0.33     | 0.08                | 0.28       |
| (1,2207) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 3                   | 0.33     | 0.08                | 0.28       |
| (1,2207) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 3                   | 0.33     | 0.08                | 0.28       |
| (1,2207) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 3                   | 0.33     | 0.08                | 0.28       |
| (1,826)  | 1:139:A:THR:HA   | 1:140:A:ARG:HB2  | 3                   | 0.33     | 0.04                | 0.35       |
| (1,847)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HE3  | 3                   | 0.33     | 0.03                | 0.34       |
| (1,344)  | 1:108:A:GLU:HG2  | 1:123:A:LYS:HD3  | 3                   | 0.33     | 0.11                | 0.25       |
| (1,344)  | 1:108:A:GLU:HG2  | 1:123:A:LYS:HD2  | 3                   | 0.33     | 0.11                | 0.25       |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG21 | 3                   | 0.32     | 0.05                | 0.29       |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG22 | 3                   | 0.32     | 0.05                | 0.29       |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG23 | 3                   | 0.32     | 0.05                | 0.29       |
| (1,3304) | 1:149:B:ASP:HA   | 1:149:B:ASP:HB3  | 3                   | 0.32     | 0.1                 | 0.35       |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD21 | 3                   | 0.32     | 0.07                | 0.29       |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD22 | 3                   | 0.32     | 0.07                | 0.29       |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD23 | 3                   | 0.32     | 0.07                | 0.29       |
| (1,1321) | 1:94:A:ARG:H     | 1:93:A:ASP:HA    | 3                   | 0.31     | 0.06                | 0.34       |
| (1,1514) | 1:118:A:VAL:H    | 1:119:A:GLU:HG3  | 3                   | 0.31     | 0.16                | 0.21       |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG21 | 3                   | 0.3      | 0.11                | 0.23       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG22 | 3                   | 0.3      | 0.11                | 0.23       |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG23 | 3                   | 0.3      | 0.11                | 0.23       |
| (1,1085) | 1:153:A:VAL:HG21 | 1:155:A:SER:HB3  | 3                   | 0.3      | 0.11                | 0.31       |
| (1,1085) | 1:153:A:VAL:HG22 | 1:155:A:SER:HB3  | 3                   | 0.3      | 0.11                | 0.31       |
| (1,1085) | 1:153:A:VAL:HG23 | 1:155:A:SER:HB3  | 3                   | 0.3      | 0.11                | 0.31       |
| (1,1085) | 1:153:A:VAL:HG11 | 1:155:A:SER:HB3  | 3                   | 0.3      | 0.11                | 0.31       |
| (1,1085) | 1:153:A:VAL:HG12 | 1:155:A:SER:HB3  | 3                   | 0.3      | 0.11                | 0.31       |
| (1,1085) | 1:153:A:VAL:HG13 | 1:155:A:SER:HB3  | 3                   | 0.3      | 0.11                | 0.31       |
| (1,4037) | 1:148:B:VAL:H    | 1:170:B:PRO:HG3  | 3                   | 0.3      | 0.14                | 0.39       |
| (1,2626) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HE2  | 3                   | 0.29     | 0.07                | 0.3        |
| (1,2626) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HE3  | 3                   | 0.29     | 0.07                | 0.3        |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG21 | 3                   | 0.29     | 0.12                | 0.36       |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG22 | 3                   | 0.29     | 0.12                | 0.36       |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG23 | 3                   | 0.29     | 0.12                | 0.36       |
| (1,336)  | 1:108:A:GLU:HA   | 1:108:A:GLU:HG2  | 3                   | 0.29     | 0.05                | 0.28       |
| (1,3060) | 1:131:B:HIS:HA   | 1:131:B:HIS:HE1  | 3                   | 0.29     | 0.08                | 0.33       |
| (1,1179) | 1:157:A:LEU:HD21 | 1:163:A:LEU:HB3  | 3                   | 0.28     | 0.03                | 0.26       |
| (1,1179) | 1:157:A:LEU:HD22 | 1:163:A:LEU:HB3  | 3                   | 0.28     | 0.03                | 0.26       |
| (1,1179) | 1:157:A:LEU:HD23 | 1:163:A:LEU:HB3  | 3                   | 0.28     | 0.03                | 0.26       |
| (1,2686) | 1:110:B:THR:HG21 | 1:112:B:LYS:HD3  | 3                   | 0.28     | 0.04                | 0.26       |
| (1,2686) | 1:110:B:THR:HG22 | 1:112:B:LYS:HD3  | 3                   | 0.28     | 0.04                | 0.26       |
| (1,2686) | 1:110:B:THR:HG23 | 1:112:B:LYS:HD3  | 3                   | 0.28     | 0.04                | 0.26       |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD21 | 3                   | 0.28     | 0.08                | 0.23       |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD22 | 3                   | 0.28     | 0.08                | 0.23       |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD23 | 3                   | 0.28     | 0.08                | 0.23       |
| (1,808)  | 1:135:A:SER:HA   | 1:135:A:SER:HB2  | 3                   | 0.27     | 0.01                | 0.27       |
| (1,3607) | 1:94:B:ARG:H     | 1:168:B:PRO:HA   | 3                   | 0.27     | 0.12                | 0.19       |
| (1,2759) | 1:112:B:LYS:HE3  | 1:121:B:THR:HB   | 3                   | 0.27     | 0.17                | 0.19       |
| (1,2759) | 1:112:B:LYS:HE2  | 1:121:B:THR:HB   | 3                   | 0.27     | 0.17                | 0.19       |
| (1,917)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA2  | 3                   | 0.27     | 0.11                | 0.27       |
| (1,2018) | 1:97:B:VAL:HG21  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2018) | 1:97:B:VAL:HG22  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2018) | 1:97:B:VAL:HG23  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2018) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2018) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2018) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2150) | 1:97:B:VAL:HG21  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2150) | 1:97:B:VAL:HG22  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2150) | 1:97:B:VAL:HG23  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2150) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2150) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |
| (1,2150) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB3  | 3                   | 0.27     | 0.05                | 0.26       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2629) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HE3  | 3                   | 0.27     | 0.11                | 0.34       |
| (1,2629) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HE2  | 3                   | 0.27     | 0.11                | 0.34       |
| (1,478)  | 1:112:A:LYS:HE2  | 1:121:A:THR:HB   | 3                   | 0.26     | 0.07                | 0.26       |
| (1,478)  | 1:112:A:LYS:HE3  | 1:121:A:THR:HB   | 3                   | 0.26     | 0.07                | 0.26       |
| (1,3395) | 1:155:B:SER:HB2  | 1:163:B:LEU:HA   | 3                   | 0.26     | 0.11                | 0.27       |
| (1,4281) | 1:169:B:MET:H    | 1:169:B:MET:HG3  | 3                   | 0.25     | 0.05                | 0.25       |
| (1,2957) | 1:122:B:GLY:HA3  | 1:137:B:CYS:HA   | 3                   | 0.25     | 0.14                | 0.18       |
| (1,4191) | 1:161:B:GLY:H    | 1:160:B:GLU:HG3  | 3                   | 0.25     | 0.08                | 0.23       |
| (1,4191) | 1:161:B:GLY:H    | 1:160:B:GLU:HG2  | 3                   | 0.25     | 0.08                | 0.23       |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD11 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD12 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD13 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD11 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD12 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD13 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD11 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD12 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD13 | 3                   | 0.25     | 0.12                | 0.18       |
| (1,3027) | 1:128:B:GLN:HA   | 1:128:B:GLN:HG3  | 3                   | 0.24     | 0.16                | 0.17       |
| (1,348)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HE3  | 3                   | 0.24     | 0.12                | 0.19       |
| (1,348)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HE2  | 3                   | 0.24     | 0.12                | 0.19       |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD21 | 3                   | 0.24     | 0.0                 | 0.24       |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD22 | 3                   | 0.24     | 0.0                 | 0.24       |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD23 | 3                   | 0.24     | 0.0                 | 0.24       |
| (1,746)  | 1:128:A:GLN:HA   | 1:128:A:GLN:HG3  | 3                   | 0.24     | 0.05                | 0.2        |
| (1,2020) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 3                   | 0.24     | 0.04                | 0.26       |
| (1,2020) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 3                   | 0.24     | 0.04                | 0.26       |
| (1,2020) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 3                   | 0.24     | 0.04                | 0.26       |
| (1,2152) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 3                   | 0.24     | 0.04                | 0.26       |
| (1,2152) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 3                   | 0.24     | 0.04                | 0.26       |
| (1,2152) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 3                   | 0.24     | 0.04                | 0.26       |
| (1,2891) | 1:119:B:GLU:HA   | 1:141:B:LYS:HD3  | 3                   | 0.23     | 0.05                | 0.2        |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD21 | 3                   | 0.22     | 0.01                | 0.23       |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD22 | 3                   | 0.22     | 0.01                | 0.23       |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD23 | 3                   | 0.22     | 0.01                | 0.23       |
| (1,3595) | 1:170:B:PRO:HB3  | 1:170:B:PRO:HD3  | 3                   | 0.22     | 0.03                | 0.22       |
| (1,3595) | 1:170:B:PRO:HB3  | 1:170:B:PRO:HD2  | 3                   | 0.22     | 0.03                | 0.22       |
| (1,1318) | 1:171:A:LYS:HA   | 1:171:A:LYS:HD3  | 3                   | 0.22     | 0.06                | 0.23       |
| (1,1318) | 1:171:A:LYS:HA   | 1:171:A:LYS:HD2  | 3                   | 0.22     | 0.06                | 0.23       |
| (1,2894) | 1:119:B:GLU:HB3  | 1:121:B:THR:HB   | 3                   | 0.22     | 0.01                | 0.21       |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG21 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG22 | 3                   | 0.22     | 0.06                | 0.19       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG23 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG21 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG22 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG23 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG21 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG22 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG23 | 3                   | 0.22     | 0.06                | 0.19       |
| (1,862)  | 1:141:A:LYS:HG3  | 1:142:A:TYR:HB3  | 3                   | 0.21     | 0.04                | 0.24       |
| (1,749)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HE1  | 3                   | 0.21     | 0.03                | 0.2        |
| (1,749)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HE2  | 3                   | 0.21     | 0.03                | 0.2        |
| (1,3654) | 1:102:B:ASN:HD21 | 1:161:B:GLY:HA2  | 3                   | 0.21     | 0.06                | 0.21       |
| (1,3795) | 1:118:B:VAL:H    | 1:119:B:GLU:HG3  | 3                   | 0.21     | 0.01                | 0.21       |
| (1,1014) | 1:148:A:VAL:HG11 | 1:170:A:PRO:HG3  | 3                   | 0.2      | 0.02                | 0.2        |
| (1,1014) | 1:148:A:VAL:HG12 | 1:170:A:PRO:HG3  | 3                   | 0.2      | 0.02                | 0.2        |
| (1,1014) | 1:148:A:VAL:HG13 | 1:170:A:PRO:HG3  | 3                   | 0.2      | 0.02                | 0.2        |
| (1,773)  | 1:130:A:GLU:HA   | 1:130:A:GLU:HG3  | 3                   | 0.2      | 0.03                | 0.2        |
| (1,1327) | 1:94:A:ARG:H     | 1:169:A:MET:HG2  | 3                   | 0.2      | 0.06                | 0.22       |
| (1,3664) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA3  | 3                   | 0.2      | 0.03                | 0.21       |
| (1,1276) | 1:168:A:PRO:HA   | 1:169:A:MET:HG2  | 3                   | 0.19     | 0.07                | 0.18       |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD11 | 3                   | 0.19     | 0.05                | 0.18       |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD12 | 3                   | 0.19     | 0.05                | 0.18       |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD13 | 3                   | 0.19     | 0.05                | 0.18       |
| (1,700)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG3  | 3                   | 0.19     | 0.03                | 0.2        |
| (1,1383) | 1:102:A:ASN:HD22 | 1:161:A:GLY:HA3  | 3                   | 0.19     | 0.04                | 0.19       |
| (1,2716) | 1:111:B:VAL:HG21 | 1:120:B:ILE:HG13 | 3                   | 0.19     | 0.05                | 0.17       |
| (1,2716) | 1:111:B:VAL:HG22 | 1:120:B:ILE:HG13 | 3                   | 0.19     | 0.05                | 0.17       |
| (1,2716) | 1:111:B:VAL:HG23 | 1:120:B:ILE:HG13 | 3                   | 0.19     | 0.05                | 0.17       |
| (1,2716) | 1:111:B:VAL:HG11 | 1:120:B:ILE:HG13 | 3                   | 0.19     | 0.05                | 0.17       |
| (1,2716) | 1:111:B:VAL:HG12 | 1:120:B:ILE:HG13 | 3                   | 0.19     | 0.05                | 0.17       |
| (1,2716) | 1:111:B:VAL:HG13 | 1:120:B:ILE:HG13 | 3                   | 0.19     | 0.05                | 0.17       |
| (1,3663) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA2  | 3                   | 0.19     | 0.02                | 0.18       |
| (1,558)  | 1:117:A:VAL:HG11 | 1:141:A:LYS:HE2  | 3                   | 0.19     | 0.02                | 0.18       |
| (1,558)  | 1:117:A:VAL:HG12 | 1:141:A:LYS:HE2  | 3                   | 0.19     | 0.02                | 0.18       |
| (1,558)  | 1:117:A:VAL:HG13 | 1:141:A:LYS:HE2  | 3                   | 0.19     | 0.02                | 0.18       |
| (1,737)  | 1:127:A:ARG:HA   | 1:127:A:ARG:HD3  | 3                   | 0.18     | 0.05                | 0.21       |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD11 | 3                   | 0.18     | 0.03                | 0.19       |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD12 | 3                   | 0.18     | 0.03                | 0.19       |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD13 | 3                   | 0.18     | 0.03                | 0.19       |
| (1,2310) | 1:94:B:ARG:HA    | 1:168:B:PRO:HA   | 3                   | 0.18     | 0.04                | 0.18       |
| (1,4196) | 1:162:B:THR:H    | 1:102:B:ASN:HB2  | 3                   | 0.18     | 0.04                | 0.18       |
| (1,1545) | 1:120:A:ILE:H    | 1:140:A:ARG:HG3  | 3                   | 0.18     | 0.04                | 0.2        |
| (1,2330) | 1:94:B:ARG:HD3   | 1:168:B:PRO:HA   | 3                   | 0.18     | 0.09                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2518) | 1:99:B:LEU:HD21  | 1:101:B:VAL:HB   | 3                   | 0.18     | 0.01                | 0.17       |
| (1,2518) | 1:99:B:LEU:HD22  | 1:101:B:VAL:HB   | 3                   | 0.18     | 0.01                | 0.17       |
| (1,2518) | 1:99:B:LEU:HD23  | 1:101:B:VAL:HB   | 3                   | 0.18     | 0.01                | 0.17       |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE1  | 3                   | 0.18     | 0.04                | 0.15       |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE2  | 3                   | 0.18     | 0.04                | 0.15       |
| (1,1489) | 1:114:A:LYS:H    | 1:119:A:GLU:H    | 3                   | 0.17     | 0.02                | 0.17       |
| (1,226)  | 1:99:A:LEU:HD11  | 1:101:A:VAL:HG21 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD11  | 1:101:A:VAL:HG22 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD11  | 1:101:A:VAL:HG23 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD12  | 1:101:A:VAL:HG21 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD12  | 1:101:A:VAL:HG22 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD12  | 1:101:A:VAL:HG23 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD13  | 1:101:A:VAL:HG21 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD13  | 1:101:A:VAL:HG22 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,226)  | 1:99:A:LEU:HD13  | 1:101:A:VAL:HG23 | 3                   | 0.17     | 0.06                | 0.13       |
| (1,849)  | 1:141:A:LYS:HB2  | 1:141:A:LYS:HE2  | 3                   | 0.17     | 0.03                | 0.18       |
| (1,3133) | 1:141:B:LYS:HG2  | 1:141:B:LYS:HE2  | 3                   | 0.17     | 0.03                | 0.17       |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG11 | 3                   | 0.16     | 0.04                | 0.15       |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG12 | 3                   | 0.16     | 0.04                | 0.15       |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG13 | 3                   | 0.16     | 0.04                | 0.15       |
| (1,2361) | 1:96:B:ARG:HA    | 1:96:B:ARG:HD3   | 3                   | 0.16     | 0.01                | 0.15       |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD11 | 3                   | 0.16     | 0.02                | 0.15       |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD12 | 3                   | 0.16     | 0.02                | 0.15       |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD13 | 3                   | 0.16     | 0.02                | 0.15       |
| (1,1373) | 1:102:A:ASN:HD21 | 1:161:A:GLY:HA2  | 3                   | 0.16     | 0.02                | 0.15       |
| (1,1581) | 1:125:A:GLU:H    | 1:108:A:GLU:HG3  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,1611) | 1:128:A:GLN:HE22 | 1:128:A:GLN:H    | 3                   | 0.16     | 0.04                | 0.15       |
| (1,2028) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 3                   | 0.16     | 0.0                 | 0.16       |
| (1,2160) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 3                   | 0.16     | 0.0                 | 0.16       |
| (1,331)  | 1:107:A:ASP:HA   | 1:108:A:GLU:HG2  | 3                   | 0.15     | 0.02                | 0.16       |
| (1,649)  | 1:120:A:ILE:HG21 | 1:140:A:ARG:HA   | 3                   | 0.15     | 0.07                | 0.11       |
| (1,649)  | 1:120:A:ILE:HG22 | 1:140:A:ARG:HA   | 3                   | 0.15     | 0.07                | 0.11       |
| (1,649)  | 1:120:A:ILE:HG23 | 1:140:A:ARG:HA   | 3                   | 0.15     | 0.07                | 0.11       |
| (1,766)  | 1:129:A:ASP:HA   | 1:130:A:GLU:HB2  | 3                   | 0.15     | 0.03                | 0.14       |
| (1,766)  | 1:129:A:ASP:HA   | 1:130:A:GLU:HB3  | 3                   | 0.15     | 0.03                | 0.14       |
| (1,1925) | 1:162:A:THR:H    | 1:160:A:GLU:HG3  | 3                   | 0.15     | 0.03                | 0.14       |
| (1,1925) | 1:162:A:THR:H    | 1:160:A:GLU:HG2  | 3                   | 0.15     | 0.03                | 0.14       |
| (1,101)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HA   | 3                   | 0.15     | 0.03                | 0.16       |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD11 | 3                   | 0.15     | 0.04                | 0.14       |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD12 | 3                   | 0.15     | 0.04                | 0.14       |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD13 | 3                   | 0.15     | 0.04                | 0.14       |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB1  | 3                   | 0.15     | 0.03                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB2  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB3  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1389) | 1:105:A:ALA:H    | 1:106:A:PRO:HD3  | 3                   | 0.14     | 0.02                | 0.15       |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD1  | 3                   | 0.14     | 0.03                | 0.13       |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD2  | 3                   | 0.14     | 0.03                | 0.13       |
| (1,3869) | 1:126:B:GLU:H    | 1:125:B:GLU:HG3  | 3                   | 0.14     | 0.02                | 0.14       |
| (1,779)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HE1  | 3                   | 0.14     | 0.02                | 0.15       |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD11 | 3                   | 0.14     | 0.05                | 0.11       |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD12 | 3                   | 0.14     | 0.05                | 0.11       |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD13 | 3                   | 0.14     | 0.05                | 0.11       |
| (1,1576) | 1:124:A:HIS:H    | 1:136:A:ARG:HA   | 3                   | 0.14     | 0.04                | 0.11       |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 3                   | 0.14     | 0.03                | 0.12       |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 3                   | 0.14     | 0.03                | 0.12       |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 3                   | 0.14     | 0.03                | 0.12       |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 3                   | 0.14     | 0.03                | 0.12       |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 3                   | 0.14     | 0.03                | 0.12       |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 3                   | 0.14     | 0.03                | 0.12       |
| (1,992)  | 1:148:A:VAL:HA   | 1:170:A:PRO:HB3  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,3455) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HG   | 3                   | 0.13     | 0.03                | 0.12       |
| (1,3455) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HG   | 3                   | 0.13     | 0.03                | 0.12       |
| (1,3455) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HG   | 3                   | 0.13     | 0.03                | 0.12       |
| (1,4278) | 1:169:B:MET:H    | 1:169:B:MET:HA   | 3                   | 0.13     | 0.02                | 0.14       |
| (1,3453) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB2  | 3                   | 0.13     | 0.02                | 0.14       |
| (1,3453) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB2  | 3                   | 0.13     | 0.02                | 0.14       |
| (1,3453) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB2  | 3                   | 0.13     | 0.02                | 0.14       |
| (1,236)  | 1:99:A:LEU:HD11  | 1:164:A:THR:HA   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,236)  | 1:99:A:LEU:HD12  | 1:164:A:THR:HA   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,236)  | 1:99:A:LEU:HD13  | 1:164:A:THR:HA   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,571)  | 1:118:A:VAL:HB   | 1:142:A:TYR:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,571)  | 1:118:A:VAL:HB   | 1:142:A:TYR:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2304) | 1:94:B:ARG:HA    | 1:94:B:ARG:HB3   | 3                   | 0.13     | 0.02                | 0.13       |
| (1,161)  | 1:97:A:VAL:HG21  | 1:166:A:GLU:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,161)  | 1:97:A:VAL:HG22  | 1:166:A:GLU:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,161)  | 1:97:A:VAL:HG23  | 1:166:A:GLU:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1668) | 1:135:A:SER:H    | 1:135:A:SER:HB3  | 3                   | 0.12     | 0.03                | 0.11       |
| (1,1870) | 1:157:A:LEU:H    | 1:157:A:LEU:HB3  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,2798) | 1:115:B:ASP:HB3  | 1:150:B:PRO:HG2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG21 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG22 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG23 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,4043) | 1:149:B:ASP:H    | 1:152:B:GLN:HB2  | 3                   | 0.12     | 0.01                | 0.13       |
| (1,759)  | 1:128:A:GLN:HG2  | 1:133:A:TYR:HA   | 3                   | 0.12     | 0.01                | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1849) | 1:155:A:SER:H    | 1:156:A:SER:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,143)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE1  | 3                   | 0.11     | 0.02                | 0.1        |
| (1,143)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE2  | 3                   | 0.11     | 0.02                | 0.1        |
| (1,143)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE1  | 3                   | 0.11     | 0.02                | 0.1        |
| (1,143)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE2  | 3                   | 0.11     | 0.02                | 0.1        |
| (1,143)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE1  | 3                   | 0.11     | 0.02                | 0.1        |
| (1,143)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE2  | 3                   | 0.11     | 0.02                | 0.1        |
| (1,2885) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG12 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,719)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD1  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,719)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2302) | 1:93:B:ASP:HB3   | 1:94:B:ARG:HG2   | 2                   | 1.48     | 0.17                | 1.48       |
| (1,1614) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB2  | 2                   | 0.9      | 0.23                | 0.9        |
| (1,2012) | 1:172:A:LEU:H    | 1:171:A:LYS:HA   | 2                   | 0.9      | 0.07                | 0.9        |
| (1,3271) | 1:148:B:VAL:HA   | 1:169:B:MET:HB2  | 2                   | 0.87     | 0.11                | 0.87       |
| (1,3293) | 1:148:B:VAL:HG11 | 1:169:B:MET:HB2  | 2                   | 0.7      | 0.14                | 0.7        |
| (1,3293) | 1:148:B:VAL:HG12 | 1:169:B:MET:HB2  | 2                   | 0.7      | 0.14                | 0.7        |
| (1,3293) | 1:148:B:VAL:HG13 | 1:169:B:MET:HB2  | 2                   | 0.7      | 0.14                | 0.7        |
| (1,1482) | 1:114:A:LYS:H    | 1:115:A:ASP:HB2  | 2                   | 0.62     | 0.19                | 0.62       |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG21  | 2                   | 0.58     | 0.41                | 0.58       |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG22  | 2                   | 0.58     | 0.41                | 0.58       |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG23  | 2                   | 0.58     | 0.41                | 0.58       |
| (1,2545) | 1:100:B:ASP:HB2  | 1:162:B:THR:HB   | 2                   | 0.56     | 0.13                | 0.56       |
| (1,4065) | 1:152:B:GLN:H    | 1:149:B:ASP:HB3  | 2                   | 0.55     | 0.24                | 0.55       |
| (1,4086) | 1:152:B:GLN:HE21 | 1:170:B:PRO:HD3  | 2                   | 0.53     | 0.35                | 0.53       |
| (1,2991) | 1:126:B:GLU:HA   | 1:135:B:SER:HB2  | 2                   | 0.52     | 0.29                | 0.52       |
| (1,770)  | 1:129:A:ASP:HB3  | 1:130:A:GLU:HA   | 2                   | 0.52     | 0.04                | 0.52       |
| (1,345)  | 1:108:A:GLU:HG2  | 1:123:A:LYS:HE2  | 2                   | 0.46     | 0.01                | 0.46       |
| (1,1608) | 1:128:A:GLN:HE22 | 1:128:A:GLN:HB2  | 2                   | 0.46     | 0.27                | 0.46       |
| (1,834)  | 1:139:A:THR:HG21 | 1:140:A:ARG:HG3  | 2                   | 0.46     | 0.01                | 0.46       |
| (1,834)  | 1:139:A:THR:HG22 | 1:140:A:ARG:HG3  | 2                   | 0.46     | 0.01                | 0.46       |
| (1,834)  | 1:139:A:THR:HG23 | 1:140:A:ARG:HG3  | 2                   | 0.46     | 0.01                | 0.46       |
| (1,2287) | 1:90:B:HIS:HA    | 1:91:B:THR:HG21  | 2                   | 0.46     | 0.18                | 0.46       |
| (1,2287) | 1:90:B:HIS:HA    | 1:91:B:THR:HG22  | 2                   | 0.46     | 0.18                | 0.46       |
| (1,2287) | 1:90:B:HIS:HA    | 1:91:B:THR:HG23  | 2                   | 0.46     | 0.18                | 0.46       |
| (1,2068) | 1:134:B:ILE:HG21 | 1:140:A:ARG:HD3  | 2                   | 0.43     | 0.09                | 0.43       |
| (1,2068) | 1:134:B:ILE:HG22 | 1:140:A:ARG:HD3  | 2                   | 0.43     | 0.09                | 0.43       |
| (1,2068) | 1:134:B:ILE:HG23 | 1:140:A:ARG:HD3  | 2                   | 0.43     | 0.09                | 0.43       |
| (1,2200) | 1:134:B:ILE:HG21 | 1:140:A:ARG:HD3  | 2                   | 0.43     | 0.09                | 0.43       |
| (1,2200) | 1:134:B:ILE:HG22 | 1:140:A:ARG:HD3  | 2                   | 0.43     | 0.09                | 0.43       |
| (1,2200) | 1:134:B:ILE:HG23 | 1:140:A:ARG:HD3  | 2                   | 0.43     | 0.09                | 0.43       |
| (1,1920) | 1:162:A:THR:H    | 1:158:A:SER:HB2  | 2                   | 0.42     | 0.24                | 0.42       |
| (1,2008) | 1:171:A:LYS:H    | 1:171:A:LYS:HA   | 2                   | 0.42     | 0.01                | 0.42       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2313) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD3  | 2                   | 0.41     | 0.14                | 0.41       |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD21 | 2                   | 0.4      | 0.02                | 0.4        |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD22 | 2                   | 0.4      | 0.02                | 0.4        |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD23 | 2                   | 0.4      | 0.02                | 0.4        |
| (1,2013) | 1:172:A:LEU:H    | 1:172:A:LEU:HB2  | 2                   | 0.39     | 0.22                | 0.39       |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG21 | 2                   | 0.38     | 0.05                | 0.38       |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG22 | 2                   | 0.38     | 0.05                | 0.38       |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG23 | 2                   | 0.38     | 0.05                | 0.38       |
| (1,1656) | 1:134:A:ILE:H    | 1:127:A:ARG:HG3  | 2                   | 0.36     | 0.24                | 0.36       |
| (1,4036) | 1:148:B:VAL:H    | 1:170:B:PRO:HB2  | 2                   | 0.35     | 0.19                | 0.35       |
| (1,247)  | 1:99:A:LEU:HD21  | 1:140:A:ARG:HG3  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,247)  | 1:99:A:LEU:HD22  | 1:140:A:ARG:HG3  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,247)  | 1:99:A:LEU:HD23  | 1:140:A:ARG:HG3  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,3492) | 1:160:B:GLU:HG2  | 1:162:B:THR:HB   | 2                   | 0.34     | 0.02                | 0.34       |
| (1,4290) | 1:171:B:LYS:H    | 1:171:B:LYS:HB3  | 2                   | 0.34     | 0.01                | 0.34       |
| (1,4290) | 1:171:B:LYS:H    | 1:171:B:LYS:HB2  | 2                   | 0.34     | 0.01                | 0.34       |
| (1,472)  | 1:112:A:LYS:HD2  | 1:120:A:ILE:HA   | 2                   | 0.33     | 0.12                | 0.33       |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD21 | 2                   | 0.33     | 0.01                | 0.33       |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD22 | 2                   | 0.33     | 0.01                | 0.33       |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD23 | 2                   | 0.33     | 0.01                | 0.33       |
| (1,3889) | 1:128:B:GLN:HE22 | 1:128:B:GLN:HB2  | 2                   | 0.33     | 0.18                | 0.33       |
| (1,1767) | 1:149:A:ASP:H    | 1:170:A:PRO:HG3  | 2                   | 0.32     | 0.13                | 0.32       |
| (1,2529) | 1:99:B:LEU:HD21  | 1:140:B:ARG:HD2  | 2                   | 0.32     | 0.06                | 0.32       |
| (1,2529) | 1:99:B:LEU:HD22  | 1:140:B:ARG:HD2  | 2                   | 0.32     | 0.06                | 0.32       |
| (1,2529) | 1:99:B:LEU:HD23  | 1:140:B:ARG:HD2  | 2                   | 0.32     | 0.06                | 0.32       |
| (1,1323) | 1:94:A:ARG:H     | 1:93:A:ASP:HB3   | 2                   | 0.3      | 0.01                | 0.3        |
| (1,1326) | 1:94:A:ARG:H     | 1:168:A:PRO:HA   | 2                   | 0.3      | 0.08                | 0.3        |
| (1,1805) | 1:152:A:GLN:HE21 | 1:170:A:PRO:HD3  | 2                   | 0.29     | 0.05                | 0.29       |
| (1,3602) | 1:94:B:ARG:H     | 1:93:B:ASP:HA    | 2                   | 0.29     | 0.03                | 0.29       |
| (1,338)  | 1:108:A:GLU:HA   | 1:123:A:LYS:HD2  | 2                   | 0.29     | 0.06                | 0.29       |
| (1,3862) | 1:125:B:GLU:H    | 1:108:B:GLU:HG3  | 2                   | 0.29     | 0.02                | 0.29       |
| (1,1915) | 1:162:A:THR:H    | 1:102:A:ASN:HB2  | 2                   | 0.28     | 0.02                | 0.28       |
| (1,19)   | 1:93:A:ASP:HB2   | 1:94:A:ARG:HG2   | 2                   | 0.28     | 0.02                | 0.28       |
| (1,3014) | 1:126:B:GLU:HG3  | 1:135:B:SER:HB3  | 2                   | 0.28     | 0.1                 | 0.28       |
| (1,264)  | 1:100:A:ASP:HB2  | 1:162:A:THR:HB   | 2                   | 0.26     | 0.12                | 0.26       |
| (1,635)  | 1:120:A:ILE:HB   | 1:140:A:ARG:HD2  | 2                   | 0.26     | 0.06                | 0.26       |
| (1,1650) | 1:132:A:GLY:H    | 1:133:A:TYR:HD1  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,1650) | 1:132:A:GLY:H    | 1:133:A:TYR:HD2  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,3120) | 1:140:B:ARG:HB2  | 1:140:B:ARG:HD2  | 2                   | 0.26     | 0.07                | 0.26       |
| (1,2060) | 1:134:B:ILE:HA   | 1:140:A:ARG:HG3  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,2192) | 1:134:B:ILE:HA   | 1:140:A:ARG:HG3  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,3599) | 1:171:B:LYS:HA   | 1:171:B:LYS:HD2  | 2                   | 0.25     | 0.04                | 0.25       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3599) | 1:171:B:LYS:HA   | 1:171:B:LYS:HD3  | 2                   | 0.25     | 0.04                | 0.25       |
| (1,703)  | 1:125:A:GLU:HA   | 1:135:A:SER:HB2  | 2                   | 0.24     | 0.08                | 0.24       |
| (1,2754) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB2  | 2                   | 0.24     | 0.11                | 0.24       |
| (1,2754) | 1:112:B:LYS:HE3  | 1:114:B:LYS:HB2  | 2                   | 0.24     | 0.11                | 0.24       |
| (1,3865) | 1:125:B:GLU:H    | 1:126:B:GLU:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,2965) | 1:123:B:LYS:HA   | 1:135:B:SER:HB3  | 2                   | 0.24     | 0.02                | 0.24       |
| (1,3500) | 1:162:B:THR:HA   | 1:162:B:THR:HG21 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,3500) | 1:162:B:THR:HA   | 1:162:B:THR:HG22 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,3500) | 1:162:B:THR:HA   | 1:162:B:THR:HG23 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,3908) | 1:129:B:ASP:H    | 1:132:B:GLY:H    | 2                   | 0.24     | 0.02                | 0.24       |
| (1,69)   | 1:95:A:TRP:HB3   | 1:166:A:GLU:HB2  | 2                   | 0.23     | 0.11                | 0.23       |
| (1,1584) | 1:125:A:GLU:H    | 1:126:A:GLU:H    | 2                   | 0.23     | 0.04                | 0.23       |
| (1,3366) | 1:153:B:VAL:HG11 | 1:155:B:SER:HB3  | 2                   | 0.23     | 0.0                 | 0.23       |
| (1,3366) | 1:153:B:VAL:HG12 | 1:155:B:SER:HB3  | 2                   | 0.23     | 0.0                 | 0.23       |
| (1,3366) | 1:153:B:VAL:HG13 | 1:155:B:SER:HB3  | 2                   | 0.23     | 0.0                 | 0.23       |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG11 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG12 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG13 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,4052) | 1:151:B:THR:H    | 1:149:B:ASP:HB3  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,1191) | 1:158:A:SER:HB2  | 1:160:A:GLU:HG2  | 2                   | 0.22     | 0.06                | 0.22       |
| (1,1910) | 1:161:A:GLY:H    | 1:160:A:GLU:HG3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,3861) | 1:125:B:GLU:H    | 1:108:B:GLU:HG2  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD21 | 2                   | 0.21     | 0.05                | 0.21       |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD22 | 2                   | 0.21     | 0.05                | 0.21       |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD23 | 2                   | 0.21     | 0.05                | 0.21       |
| (1,2592) | 1:106:B:PRO:HA   | 1:109:B:LEU:HB2  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,2981) | 1:125:B:GLU:HA   | 1:125:B:GLU:HG3  | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,3672) | 1:105:B:ALA:H    | 1:108:B:GLU:HB3  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,2613) | 1:107:B:ASP:HA   | 1:108:B:GLU:HG3  | 2                   | 0.2      | 0.07                | 0.2        |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD11 | 2                   | 0.2      | 0.02                | 0.2        |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD12 | 2                   | 0.2      | 0.02                | 0.2        |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD13 | 2                   | 0.2      | 0.02                | 0.2        |
| (1,756)  | 1:128:A:GLN:HB3  | 1:133:A:TYR:HD1  | 2                   | 0.2      | 0.04                | 0.2        |
| (1,756)  | 1:128:A:GLN:HB3  | 1:133:A:TYR:HD2  | 2                   | 0.2      | 0.04                | 0.2        |
| (1,3868) | 1:126:B:GLU:H    | 1:125:B:GLU:HG2  | 2                   | 0.19     | 0.01                | 0.19       |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD21  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD22  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD23  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,717)  | 1:126:A:GLU:HG2  | 1:127:A:ARG:HG3  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,883)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG21 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,883)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG22 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,883)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG23 | 2                   | 0.18     | 0.04                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,883)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG21 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,883)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG22 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,883)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG23 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:105:A:ALA:HB1  | 1:107:A:ASP:HB2  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,296)  | 1:105:A:ALA:HB2  | 1:107:A:ASP:HB2  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,296)  | 1:105:A:ALA:HB3  | 1:107:A:ASP:HB2  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,1104) | 1:155:A:SER:HA   | 1:156:A:SER:HB3  | 2                   | 0.18     | 0.01                | 0.18       |
| (1,3759) | 1:114:B:LYS:H    | 1:112:B:LYS:HD3  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,1733) | 1:147:A:GLY:H    | 1:146:A:PRO:HG2  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,2540) | 1:100:B:ASP:HA   | 1:100:B:ASP:HB3  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,3000) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HD1  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,3000) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HD2  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,4115) | 1:154:B:SER:H    | 1:155:B:SER:HB2  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,4194) | 1:161:B:GLY:H    | 1:162:B:THR:HB   | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,602)  | 1:119:A:GLU:HA   | 1:119:A:GLU:HG3  | 2                   | 0.17     | 0.0                 | 0.17       |
| (1,1643) | 1:132:A:GLY:H    | 1:130:A:GLU:HB2  | 2                   | 0.17     | 0.06                | 0.17       |
| (1,1643) | 1:132:A:GLY:H    | 1:130:A:GLU:HB3  | 2                   | 0.17     | 0.06                | 0.17       |
| (1,2749) | 1:112:B:LYS:HG2  | 1:121:B:THR:HB   | 2                   | 0.17     | 0.06                | 0.17       |
| (1,610)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HD3  | 2                   | 0.17     | 0.02                | 0.17       |
| (1,1844) | 1:154:A:SER:H    | 1:168:A:PRO:HD2  | 2                   | 0.17     | 0.05                | 0.17       |
| (1,2559) | 1:102:B:ASN:HB2  | 1:161:B:GLY:HA3  | 2                   | 0.17     | 0.04                | 0.17       |
| (1,4125) | 1:154:B:SER:H    | 1:168:B:PRO:HD2  | 2                   | 0.17     | 0.01                | 0.17       |
| (1,751)  | 1:128:A:GLN:HA   | 1:134:A:ILE:HD11 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,751)  | 1:128:A:GLN:HA   | 1:134:A:ILE:HD12 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,751)  | 1:128:A:GLN:HA   | 1:134:A:ILE:HD13 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,3093) | 1:136:B:ARG:HA   | 1:136:B:ARG:HD2  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD11 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD12 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD13 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,3481) | 1:159:B:PRO:HA   | 1:159:B:PRO:HG3  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,248)  | 1:99:A:LEU:HD21  | 1:140:A:ARG:HD2  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,248)  | 1:99:A:LEU:HD22  | 1:140:A:ARG:HD2  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,248)  | 1:99:A:LEU:HD23  | 1:140:A:ARG:HD2  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,298)  | 1:105:A:ALA:HB1  | 1:108:A:GLU:HB2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,298)  | 1:105:A:ALA:HB2  | 1:108:A:GLU:HB2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,298)  | 1:105:A:ALA:HB3  | 1:108:A:GLU:HB2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1606) | 1:128:A:GLN:H    | 1:133:A:TYR:HD1  | 2                   | 0.15     | 0.01                | 0.15       |
| (1,1606) | 1:128:A:GLN:H    | 1:133:A:TYR:HD2  | 2                   | 0.15     | 0.01                | 0.15       |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB1  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,1958) | 1:165:A:VAL:H    | 1:166:A:GLU:HB3  | 2                   | 0.15     | 0.04                | 0.15       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3903) | 1:129:B:ASP:H    | 1:129:B:ASP:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,29)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HA   | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD21 | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD22 | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD23 | 2                   | 0.15     | 0.02                | 0.15       |
| (1,938)  | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG21 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG22 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG23 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG21 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG22 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG23 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG21 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG22 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,938)  | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG23 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,764)  | 1:129:A:ASP:HA   | 1:129:A:ASP:HB3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1382) | 1:102:A:ASN:HD22 | 1:161:A:GLY:HA2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,2883) | 1:119:B:GLU:HA   | 1:119:B:GLU:HG3  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,3479) | 1:159:B:PRO:HA   | 1:159:B:PRO:HB3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,3608) | 1:94:B:ARG:H     | 1:169:B:MET:HG2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,60)   | 1:95:A:TRP:HB2   | 1:95:A:TRP:HE3   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,590)  | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1174) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HG   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1174) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HG   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1174) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HG   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1669) | 1:136:A:ARG:H    | 1:134:A:ILE:HG21 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1669) | 1:136:A:ARG:H    | 1:134:A:ILE:HG22 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1669) | 1:136:A:ARG:H    | 1:134:A:ILE:HG23 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,2357) | 1:95:B:TRP:HE3   | 1:166:B:GLU:HA   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,3498) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HA   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,812)  | 1:136:A:ARG:HA   | 1:136:A:ARG:HD2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,852)  | 1:141:A:LYS:HG2  | 1:141:A:LYS:HE2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,1428) | 1:109:A:LEU:H    | 1:109:A:LEU:HB3  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1546) | 1:120:A:ILE:H    | 1:142:A:TYR:H    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1600) | 1:128:A:GLN:H    | 1:127:A:ARG:HD2  | 2                   | 0.13     | 0.02                | 0.13       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1622) | 1:129:A:ASP:H    | 1:129:A:ASP:HB3  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1806) | 1:152:A:GLN:HE22 | 1:149:A:ASP:HB2  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,3266) | 1:148:B:VAL:HA   | 1:149:B:ASP:HB3  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD11 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD12 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD13 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD21 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD22 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD23 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,4239) | 1:165:B:VAL:H    | 1:166:B:GLU:HB3  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,604)  | 1:119:A:GLU:HA   | 1:120:A:ILE:HG12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,608)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HA   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1762) | 1:149:A:ASP:H    | 1:152:A:GLN:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD11 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD12 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2866) | 1:118:B:VAL:HG11 | 1:142:B:TYR:HD1  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2866) | 1:118:B:VAL:HG11 | 1:142:B:TYR:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2866) | 1:118:B:VAL:HG12 | 1:142:B:TYR:HD1  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2866) | 1:118:B:VAL:HG12 | 1:142:B:TYR:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2866) | 1:118:B:VAL:HG13 | 1:142:B:TYR:HD1  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2866) | 1:118:B:VAL:HG13 | 1:142:B:TYR:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2900) | 1:119:B:GLU:HG2  | 1:141:B:LYS:HE3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3879) | 1:128:B:GLN:H    | 1:127:B:ARG:HG2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,4158) | 1:158:B:SER:H    | 1:109:B:LEU:HD11 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,4158) | 1:158:B:SER:H    | 1:109:B:LEU:HD12 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,4158) | 1:158:B:SER:H    | 1:109:B:LEU:HD13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,853)  | 1:141:A:LYS:HG2  | 1:141:A:LYS:HE3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1834) | 1:154:A:SER:H    | 1:155:A:SER:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2704) | 1:111:B:VAL:HB   | 1:112:B:LYS:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3278) | 1:148:B:VAL:HB   | 1:150:B:PRO:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD11 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD12 | 2                   | 0.12     | 0.01                | 0.12       |

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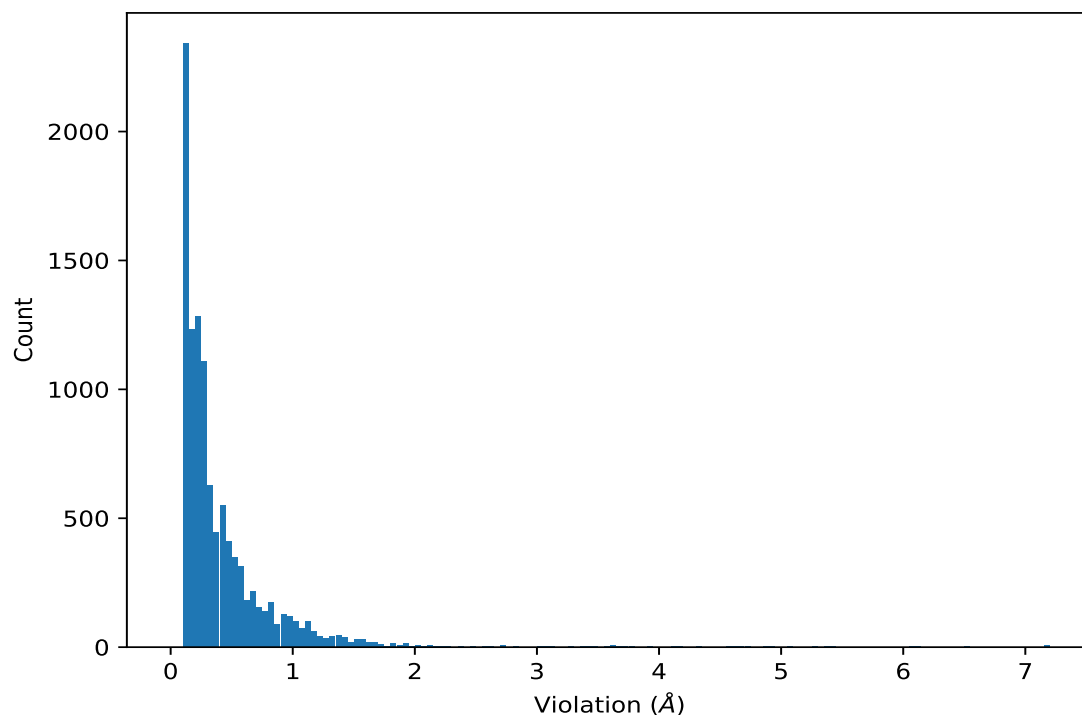
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2382) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HA   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2933) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2933) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2933) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1217) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2400) | 1:97:B:VAL:HA    | 1:97:B:VAL:HG11  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2400) | 1:97:B:VAL:HA    | 1:97:B:VAL:HG12  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2400) | 1:97:B:VAL:HA    | 1:97:B:VAL:HG13  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG21 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG23 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2023) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2023) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2155) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2155) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2291) | 1:91:B:THR:HA    | 1:91:B:THR:HB    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3723) | 1:110:B:THR:H    | 1:122:B:GLY:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,517)  | 1:115:A:ASP:HB3  | 1:150:A:PRO:HG2  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG21 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG22 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG23 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD21 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD22 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD23 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1804) | 1:152:A:GLN:HE21 | 1:169:A:MET:HA   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,288)  | 1:105:A:ALA:HA   | 1:109:A:LEU:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,288)  | 1:105:A:ALA:HA   | 1:109:A:LEU:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,288)  | 1:105:A:ALA:HA   | 1:109:A:LEU:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1616) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HG2  | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2003) | 1:171:A:LYS:H | 1:92:A:ALA:HB1  | 5        | 7.17          |
| (1,2003) | 1:171:A:LYS:H | 1:92:A:ALA:HB2  | 5        | 7.17          |
| (1,2003) | 1:171:A:LYS:H | 1:92:A:ALA:HB3  | 5        | 7.17          |
| (1,4284) | 1:171:B:LYS:H | 1:92:B:ALA:HB1  | 4        | 7.16          |
| (1,4284) | 1:171:B:LYS:H | 1:92:B:ALA:HB2  | 4        | 7.16          |
| (1,4284) | 1:171:B:LYS:H | 1:92:B:ALA:HB3  | 4        | 7.16          |
| (1,2016) | 1:174:A:THR:H | 1:171:A:LYS:HG3 | 7        | 6.94          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 5        | 6.54          |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 8        | 6.54          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 9        | 6.42          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB1  | 3        | 6.11          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB2  | 3        | 6.11          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB3  | 3        | 6.11          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB1  | 6        | 6.06          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB2  | 6        | 6.06          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB3  | 6        | 6.06          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 3        | 6.0           |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 4        | 5.86          |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 6        | 5.81          |
| (1,4283) | 1:169:B:MET:H   | 1:171:B:LYS:HE2 | 4        | 5.7           |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG3 | 3        | 5.63          |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 3        | 5.52          |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 2        | 5.46          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB1  | 8        | 5.41          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB2  | 8        | 5.41          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB3  | 8        | 5.41          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB1  | 2        | 5.36          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB2  | 2        | 5.36          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB3  | 2        | 5.36          |
| (1,3583) | 1:169:B:MET:HB2 | 1:171:B:LYS:HE2 | 10       | 5.28          |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG2 | 1        | 5.27          |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG3 | 4        | 5.23          |
| (1,4283) | 1:169:B:MET:H   | 1:171:B:LYS:HE2 | 10       | 5.1           |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG2 | 6        | 5.1           |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG2 | 10       | 5.07          |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 7        | 5.01          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1  | 9        | 4.91          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2  | 9        | 4.91          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3  | 9        | 4.91          |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 9        | 4.91          |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 10       | 4.89          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 4        | 4.86          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB1  | 9        | 4.86          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB2  | 9        | 4.86          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB3  | 9        | 4.86          |
| (1,2002) | 1:169:A:MET:H   | 1:171:A:LYS:HE3 | 5        | 4.74          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1  | 3        | 4.7           |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2  | 3        | 4.7           |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3  | 3        | 4.7           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3583) | 1:169:B:MET:HB2 | 1:171:B:LYS:HE3 | 1        | 4.68          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB1  | 5        | 4.65          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB2  | 5        | 4.65          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB3  | 5        | 4.65          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB1  | 4        | 4.64          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB2  | 4        | 4.64          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB3  | 4        | 4.64          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB1  | 1        | 4.56          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB2  | 1        | 4.56          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB3  | 1        | 4.56          |
| (1,2002) | 1:169:A:MET:H   | 1:171:A:LYS:HE2 | 4        | 4.52          |
| (1,3583) | 1:169:B:MET:HB2 | 1:171:B:LYS:HE2 | 2        | 4.44          |
| (1,1302) | 1:169:A:MET:HB2 | 1:171:A:LYS:HE2 | 4        | 4.36          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB1  | 1        | 4.3           |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB2  | 1        | 4.3           |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB3  | 1        | 4.3           |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG2 | 3        | 4.25          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1  | 8        | 4.19          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2  | 8        | 4.19          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3  | 8        | 4.19          |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG2 | 2        | 4.14          |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG2 | 8        | 4.13          |
| (1,4283) | 1:169:B:MET:H   | 1:171:B:LYS:HE2 | 1        | 4.0           |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG3 | 8        | 3.99          |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG2 | 2        | 3.93          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB1  | 10       | 3.92          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB2  | 10       | 3.92          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB3  | 10       | 3.92          |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB1  | 9        | 3.8           |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB2  | 9        | 3.8           |
| (1,4284) | 1:171:B:LYS:H   | 1:92:B:ALA:HB3  | 9        | 3.8           |
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG3 | 3        | 3.79          |
| (1,2002) | 1:169:A:MET:H   | 1:171:A:LYS:HE3 | 6        | 3.73          |
| (1,3583) | 1:169:B:MET:HB2 | 1:171:B:LYS:HE2 | 4        | 3.72          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 8        | 3.71          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1  | 2        | 3.66          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2  | 2        | 3.66          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3  | 2        | 3.66          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB1  | 8        | 3.64          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB2  | 8        | 3.64          |
| (1,2003) | 1:171:A:LYS:H   | 1:92:A:ALA:HB3  | 8        | 3.64          |
| (1,1302) | 1:169:A:MET:HB2 | 1:171:A:LYS:HE2 | 7        | 3.64          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1  | 4        | 3.63          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2  | 4        | 3.63          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3  | 4        | 3.63          |
| (1,1302) | 1:169:A:MET:HB2 | 1:171:A:LYS:HE3 | 6        | 3.62          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 2        | 3.59          |
| (1,2)    | 1:88:A:ILE:HG21 | 1:90:A:HIS:HB3  | 5        | 3.57          |
| (1,2)    | 1:88:A:ILE:HG22 | 1:90:A:HIS:HB3  | 5        | 3.57          |
| (1,2)    | 1:88:A:ILE:HG23 | 1:90:A:HIS:HB3  | 5        | 3.57          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 10       | 3.46          |
| (1,2)    | 1:88:A:ILE:HG21 | 1:90:A:HIS:HB3  | 3        | 3.45          |
| (1,2)    | 1:88:A:ILE:HG22 | 1:90:A:HIS:HB3  | 3        | 3.45          |
| (1,2)    | 1:88:A:ILE:HG23 | 1:90:A:HIS:HB3  | 3        | 3.45          |
| (1,17)   | 1:93:A:ASP:HA   | 1:169:A:MET:HG2 | 1        | 3.44          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 6        | 3.42          |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG2 | 6        | 3.4           |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 1        | 3.38          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB1  | 9        | 3.36          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB2  | 9        | 3.36          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB3  | 9        | 3.36          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1  | 7        | 3.27          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2  | 7        | 3.27          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3  | 7        | 3.27          |
| (1,3583) | 1:169:B:MET:HB2 | 1:171:B:LYS:HE2 | 3        | 3.25          |
| (1,4283) | 1:169:B:MET:H   | 1:171:B:LYS:HE2 | 2        | 3.24          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB1  | 1        | 3.14          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB2  | 1        | 3.14          |
| (1,4268) | 1:169:B:MET:H   | 1:92:B:ALA:HB3  | 1        | 3.14          |
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG2 | 10       | 3.09          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB1  | 4        | 3.07          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB2  | 4        | 3.07          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB3  | 4        | 3.07          |
| (1,2283) | 1:88:B:ILE:HG21 | 1:90:B:HIS:HB3  | 7        | 3.04          |
| (1,2283) | 1:88:B:ILE:HG22 | 1:90:B:HIS:HB3  | 7        | 3.04          |
| (1,2283) | 1:88:B:ILE:HG23 | 1:90:B:HIS:HB3  | 7        | 3.04          |
| (1,4283) | 1:169:B:MET:H   | 1:171:B:LYS:HE2 | 8        | 3.0           |
| (1,4297) | 1:174:B:THR:H   | 1:171:B:LYS:HG2 | 1        | 2.87          |
| (1,1)    | 1:88:A:ILE:HG21 | 1:90:A:HIS:HA   | 5        | 2.84          |
| (1,1)    | 1:88:A:ILE:HG22 | 1:90:A:HIS:HA   | 5        | 2.84          |
| (1,1)    | 1:88:A:ILE:HG23 | 1:90:A:HIS:HA   | 5        | 2.84          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB1  | 6        | 2.74          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB2  | 6        | 2.74          |
| (1,1987) | 1:169:A:MET:H   | 1:92:A:ALA:HB3  | 6        | 2.74          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG3 | 9        | 2.71          |
| (1,3600) | 1:94:B:ARG:H    | 1:91:B:THR:HG21 | 3        | 2.7           |
| (1,3600) | 1:94:B:ARG:H    | 1:91:B:THR:HG22 | 3        | 2.7           |
| (1,3600) | 1:94:B:ARG:H    | 1:91:B:THR:HG23 | 3        | 2.7           |
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG3 | 7        | 2.64          |
| (1,2298) | 1:93:B:ASP:HA   | 1:169:B:MET:HG2 | 4        | 2.64          |
| (1,17)   | 1:93:A:ASP:HA   | 1:169:A:MET:HG2 | 8        | 2.64          |
| (1,2016) | 1:174:A:THR:H   | 1:171:A:LYS:HG2 | 9        | 2.63          |
| (1,1302) | 1:169:A:MET:HB2 | 1:171:A:LYS:HE3 | 5        | 2.63          |
| (1,3583) | 1:169:B:MET:HB2 | 1:171:B:LYS:HE2 | 8        | 2.58          |
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG3 | 1        | 2.57          |
| (1,3600) | 1:94:B:ARG:H    | 1:91:B:THR:HG21 | 5        | 2.56          |
| (1,3600) | 1:94:B:ARG:H    | 1:91:B:THR:HG22 | 5        | 2.56          |
| (1,3600) | 1:94:B:ARG:H    | 1:91:B:THR:HG23 | 5        | 2.56          |
| (1,17)   | 1:93:A:ASP:HA   | 1:169:A:MET:HG2 | 5        | 2.47          |
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG3 | 4        | 2.45          |
| (1,4292) | 1:172:B:LEU:H   | 1:145:B:PRO:HA  | 7        | 2.41          |
| (1,2283) | 1:88:B:ILE:HG21 | 1:90:B:HIS:HB3  | 10       | 2.36          |
| (1,2283) | 1:88:B:ILE:HG22 | 1:90:B:HIS:HB3  | 10       | 2.36          |
| (1,2283) | 1:88:B:ILE:HG23 | 1:90:B:HIS:HB3  | 10       | 2.36          |
| (1,2002) | 1:169:A:MET:H   | 1:171:A:LYS:HE2 | 7        | 2.35          |
| (1,3583) | 1:169:B:MET:HB2 | 1:171:B:LYS:HE2 | 7        | 2.31          |
| (1,2285) | 1:89:B:ARG:HB2  | 1:90:B:HIS:HB3  | 6        | 2.3           |
| (1,2011) | 1:172:A:LEU:H   | 1:145:A:PRO:HA  | 1        | 2.28          |
| (1,2284) | 1:89:B:ARG:HB3  | 1:90:B:HIS:HB2  | 8        | 2.25          |
| (1,4)    | 1:89:A:ARG:HB2  | 1:90:A:HIS:HB3  | 8        | 2.25          |
| (1,2298) | 1:93:B:ASP:HA   | 1:169:B:MET:HG2 | 6        | 2.23          |
| (1,2)    | 1:88:A:ILE:HG21 | 1:90:A:HIS:HB3  | 7        | 2.23          |
| (1,2)    | 1:88:A:ILE:HG22 | 1:90:A:HIS:HB3  | 7        | 2.23          |
| (1,2)    | 1:88:A:ILE:HG23 | 1:90:A:HIS:HB3  | 7        | 2.23          |
| (1,4)    | 1:89:A:ARG:HB2  | 1:90:A:HIS:HB3  | 7        | 2.2           |
| (1,4283) | 1:169:B:MET:H   | 1:171:B:LYS:HE3 | 7        | 2.18          |
| (1,4283) | 1:169:B:MET:H   | 1:171:B:LYS:HE2 | 9        | 2.17          |
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG3 | 2        | 2.17          |
| (1,3582) | 1:169:B:MET:HB3 | 1:171:B:LYS:HG2 | 8        | 2.15          |
| (1,2285) | 1:89:B:ARG:HB2  | 1:90:B:HIS:HB3  | 2        | 2.14          |
| (1,1319) | 1:94:A:ARG:H    | 1:91:A:THR:HG21 | 3        | 2.14          |
| (1,1319) | 1:94:A:ARG:H    | 1:91:A:THR:HG22 | 3        | 2.14          |
| (1,1319) | 1:94:A:ARG:H    | 1:91:A:THR:HG23 | 3        | 2.14          |
| (1,2298) | 1:93:B:ASP:HA   | 1:169:B:MET:HG2 | 9        | 2.13          |
| (1,2002) | 1:169:A:MET:H   | 1:171:A:LYS:HE2 | 9        | 2.11          |
| (1,3)    | 1:89:A:ARG:HB3  | 1:90:A:HIS:HB2  | 10       | 2.08          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1302) | 1:169:A:MET:HB2  | 1:171:A:LYS:HE3  | 1        | 2.07          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 10       | 2.07          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 10       | 2.07          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 10       | 2.07          |
| (1,1302) | 1:169:A:MET:HB2  | 1:171:A:LYS:HE2  | 9        | 2.05          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB1   | 8        | 2.01          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB2   | 8        | 2.01          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB3   | 8        | 2.01          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD1  | 4        | 2.01          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD2  | 4        | 2.01          |
| (1,17)   | 1:93:A:ASP:HA    | 1:169:A:MET:HG2  | 10       | 1.99          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 4        | 1.98          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 4        | 1.98          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 4        | 1.98          |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD11 | 8        | 1.96          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 4        | 1.95          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 4        | 1.95          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 4        | 1.95          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB1   | 1        | 1.94          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB2   | 1        | 1.94          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB3   | 1        | 1.94          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 1        | 1.94          |
| (1,2283) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HB3   | 5        | 1.93          |
| (1,2283) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HB3   | 5        | 1.93          |
| (1,2283) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HB3   | 5        | 1.93          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB1  | 1        | 1.91          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB2  | 1        | 1.91          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB3  | 1        | 1.91          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB1   | 5        | 1.87          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB2   | 5        | 1.87          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB3   | 5        | 1.87          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 5        | 1.85          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 5        | 1.85          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 5        | 1.85          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 8        | 1.84          |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB1   | 7        | 1.84          |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB2   | 7        | 1.84          |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB3   | 7        | 1.84          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 8        | 1.84          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 1        | 1.83          |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD12 | 2        | 1.83          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB1   | 10       | 1.83          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB2   | 10       | 1.83          |
| (1,1987) | 1:169:A:MET:H    | 1:92:A:ALA:HB3   | 10       | 1.83          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 8        | 1.83          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 1        | 1.8           |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 3        | 1.8           |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 7        | 1.8           |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 7        | 1.8           |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 7        | 1.8           |
| (1,2285) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB3   | 3        | 1.79          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD23 | 4        | 1.79          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 8        | 1.78          |
| (1,3583) | 1:169:B:MET:HB2  | 1:171:B:LYS:HE2  | 9        | 1.76          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 6        | 1.74          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 6        | 1.74          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 6        | 1.74          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 10       | 1.74          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB1  | 7        | 1.73          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB2  | 7        | 1.73          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB3  | 7        | 1.73          |
| (1,4)    | 1:89:A:ARG:HB2   | 1:90:A:HIS:HB3   | 4        | 1.73          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 9        | 1.71          |
| (1,4)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB3   | 10       | 1.71          |
| (1,2298) | 1:93:B:ASP:HA    | 1:169:B:MET:HG2  | 10       | 1.7           |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD23 | 1        | 1.7           |
| (1,4)    | 1:89:A:ARG:HB2   | 1:90:A:HIS:HB3   | 6        | 1.7           |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 2        | 1.69          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 2        | 1.69          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 2        | 1.69          |
| (1,1)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HA    | 3        | 1.69          |
| (1,1)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HA    | 3        | 1.69          |
| (1,1)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HA    | 3        | 1.69          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 3        | 1.68          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 4        | 1.68          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 2        | 1.68          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 2        | 1.67          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 10       | 1.67          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 7        | 1.66          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG3  | 3        | 1.66          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD22 | 3        | 1.66          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 1        | 1.66          |
| (1,2608) | 1:106:B:PRO:HG2  | 1:157:B:LEU:HD11 | 4        | 1.65          |
| (1,2302) | 1:93:B:ASP:HB3   | 1:94:B:ARG:HG2   | 7        | 1.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2298) | 1:93:B:ASP:HA    | 1:169:B:MET:HG2  | 3        | 1.65          |
| (1,1301) | 1:169:A:MET:HB3  | 1:171:A:LYS:HG3  | 6        | 1.65          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD22 | 5        | 1.65          |
| (1,2298) | 1:93:B:ASP:HA    | 1:169:B:MET:HG2  | 5        | 1.64          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 7        | 1.64          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 4        | 1.63          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 4        | 1.63          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 6        | 1.63          |
| (1,4)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB3   | 1        | 1.62          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 3        | 1.61          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 3        | 1.61          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD21 | 3        | 1.61          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 4        | 1.61          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 3        | 1.61          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 3        | 1.6           |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD11 | 4        | 1.6           |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 7        | 1.6           |
| (1,3601) | 1:94:B:ARG:H     | 1:92:B:ALA:HA    | 7        | 1.59          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 4        | 1.59          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 4        | 1.59          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 4        | 1.59          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 4        | 1.59          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 4        | 1.59          |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 4        | 1.59          |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD11 | 7        | 1.59          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 3        | 1.59          |
| (1,4292) | 1:172:B:LEU:H    | 1:145:B:PRO:HA   | 5        | 1.58          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 9        | 1.58          |
| (1,2283) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HB3   | 1        | 1.58          |
| (1,2283) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HB3   | 1        | 1.58          |
| (1,2283) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HB3   | 1        | 1.58          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 8        | 1.58          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 10       | 1.58          |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD13 | 7        | 1.57          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 7        | 1.57          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 5        | 1.57          |
| (1,4)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB3   | 3        | 1.57          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD21 | 1        | 1.56          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 5        | 1.56          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 10       | 1.55          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 10       | 1.55          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 10       | 1.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2285) | 1:89:B:ARG:HB2   | 1:90:B:HIS:HB3   | 4        | 1.55          |
| (1,2284) | 1:89:B:ARG:HB2   | 1:90:B:HIS:HB2   | 2        | 1.55          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 5        | 1.55          |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 1        | 1.55          |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 2        | 1.55          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD22 | 9        | 1.54          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 2        | 1.54          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 6        | 1.54          |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 4        | 1.54          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 4        | 1.54          |
| (1,3)    | 1:89:A:ARG:HB2   | 1:90:A:HIS:HB2   | 8        | 1.54          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD1  | 9        | 1.53          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD2  | 9        | 1.53          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD22 | 5        | 1.53          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 4        | 1.53          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 7        | 1.53          |
| (1,2285) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB3   | 8        | 1.53          |
| (1,2157) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 8        | 1.53          |
| (1,2025) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 8        | 1.53          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD22 | 10       | 1.53          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 4        | 1.52          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD22 | 2        | 1.52          |
| (1,1320) | 1:94:A:ARG:H     | 1:92:A:ALA:HA    | 1        | 1.52          |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE1  | 3        | 1.52          |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE2  | 3        | 1.52          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 7        | 1.52          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 2        | 1.52          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD1  | 7        | 1.51          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD2  | 7        | 1.51          |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD12 | 3        | 1.51          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 4        | 1.5           |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 10       | 1.5           |
| (1,1301) | 1:169:A:MET:HB3  | 1:171:A:LYS:HG3  | 4        | 1.5           |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD11 | 2        | 1.5           |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 4        | 1.5           |
| (1,17)   | 1:93:A:ASP:HA    | 1:169:A:MET:HG2  | 6        | 1.5           |
| (1,3)    | 1:89:A:ARG:HB2   | 1:90:A:HIS:HB2   | 4        | 1.5           |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 6        | 1.49          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD21 | 8        | 1.49          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 1        | 1.49          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 10       | 1.49          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 9        | 1.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 9        | 1.48          |
| (1,2016) | 1:174:A:THR:H    | 1:171:A:LYS:HG3  | 4        | 1.48          |
| (1,2004) | 1:171:A:LYS:H    | 1:169:A:MET:HA   | 10       | 1.48          |
| (1,1654) | 1:134:A:ILE:H    | 1:127:A:ARG:HB2  | 1        | 1.48          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 1        | 1.48          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 2        | 1.47          |
| (1,2298) | 1:93:B:ASP:HA    | 1:169:B:MET:HG2  | 2        | 1.47          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 5        | 1.47          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 5        | 1.47          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 5        | 1.47          |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD11 | 6        | 1.46          |
| (1,2284) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB2   | 3        | 1.46          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 3        | 1.46          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 2        | 1.46          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 9        | 1.45          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 8        | 1.45          |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 8        | 1.45          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 8        | 1.45          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 2        | 1.45          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 2        | 1.45          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 2        | 1.45          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 2        | 1.45          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 2        | 1.45          |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 2        | 1.45          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 6        | 1.45          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 5        | 1.45          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD22 | 9        | 1.45          |
| (1,4297) | 1:174:B:THR:H    | 1:171:B:LYS:HG2  | 10       | 1.44          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 8        | 1.44          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 7        | 1.44          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 7        | 1.44          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 1        | 1.44          |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 1        | 1.44          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 1        | 1.44          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 8        | 1.44          |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD11 | 10       | 1.44          |
| (1,286)  | 1:105:A:ALA:HA   | 1:108:A:GLU:HB2  | 9        | 1.44          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 3        | 1.44          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 3        | 1.44          |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 3        | 1.44          |
| (1,16)   | 1:93:A:ASP:HA    | 1:94:A:ARG:HD2   | 5        | 1.43          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD23 | 10       | 1.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD13 | 5        | 1.42          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 9        | 1.42          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 9        | 1.42          |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 9        | 1.42          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 3        | 1.41          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD22 | 7        | 1.41          |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 10       | 1.41          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD23 | 2        | 1.41          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD21 | 7        | 1.41          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 7        | 1.41          |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB1   | 5        | 1.4           |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB2   | 5        | 1.4           |
| (1,4284) | 1:171:B:LYS:H    | 1:92:B:ALA:HB3   | 5        | 1.4           |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 5        | 1.4           |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 9        | 1.4           |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 9        | 1.4           |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD21 | 8        | 1.4           |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 5        | 1.4           |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD23 | 6        | 1.39          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 9        | 1.39          |
| (1,3005) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB3  | 4        | 1.38          |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD12 | 8        | 1.38          |
| (1,2285) | 1:89:B:ARG:HB2   | 1:90:B:HIS:HB3   | 9        | 1.38          |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 1        | 1.38          |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 1        | 1.38          |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 1        | 1.38          |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 1        | 1.38          |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 1        | 1.38          |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 1        | 1.38          |
| (1,328)  | 1:106:A:PRO:HD2  | 1:157:A:LEU:HD21 | 6        | 1.38          |
| (1,2)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HB3   | 6        | 1.38          |
| (1,2)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HB3   | 6        | 1.38          |
| (1,2)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HB3   | 6        | 1.38          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG21  | 6        | 1.37          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG22  | 6        | 1.37          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG23  | 6        | 1.37          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG21  | 10       | 1.37          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG22  | 10       | 1.37          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG23  | 10       | 1.37          |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD2  | 3        | 1.37          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 1        | 1.37          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 1        | 1.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 1        | 1.37          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE1  | 8        | 1.37          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE2  | 8        | 1.37          |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 5        | 1.36          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 10       | 1.36          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 7        | 1.36          |
| (1,3)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB2   | 1        | 1.36          |
| (1,3)    | 1:89:A:ARG:HB2   | 1:90:A:HIS:HB2   | 7        | 1.36          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 6        | 1.35          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 6        | 1.35          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 9        | 1.35          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 9        | 1.35          |
| (1,2290) | 1:90:B:HIS:HB3   | 1:91:B:THR:HA    | 7        | 1.35          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 9        | 1.35          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 1        | 1.34          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 1        | 1.34          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 1        | 1.34          |
| (1,2327) | 1:94:B:ARG:HG3   | 1:168:B:PRO:HA   | 7        | 1.34          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 8        | 1.34          |
| (1,110)  | 1:96:A:ARG:HG3   | 1:166:A:GLU:HB3  | 10       | 1.34          |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 6        | 1.33          |
| (1,2609) | 1:106:B:PRO:HD2  | 1:157:B:LEU:HD21 | 4        | 1.33          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 3        | 1.33          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 9        | 1.33          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 6        | 1.33          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 2        | 1.32          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 2        | 1.32          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 9        | 1.32          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 9        | 1.32          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 9        | 1.32          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 6        | 1.32          |
| (1,2538) | 1:99:B:LEU:HD11  | 1:112:B:LYS:HG3  | 6        | 1.32          |
| (1,2538) | 1:99:B:LEU:HD12  | 1:112:B:LYS:HG3  | 6        | 1.32          |
| (1,2538) | 1:99:B:LEU:HD13  | 1:112:B:LYS:HG3  | 6        | 1.32          |
| (1,4285) | 1:171:B:LYS:H    | 1:169:B:MET:HA   | 5        | 1.31          |
| (1,2302) | 1:93:B:ASP:HB3   | 1:94:B:ARG:HG2   | 3        | 1.31          |
| (1,2282) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HA    | 7        | 1.31          |
| (1,2282) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HA    | 7        | 1.31          |
| (1,2282) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HA    | 7        | 1.31          |
| (1,2002) | 1:169:A:MET:H    | 1:171:A:LYS:HE2  | 3        | 1.31          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 8        | 1.31          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 8        | 1.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 8        | 1.31          |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 2        | 1.3           |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 2        | 1.3           |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 3        | 1.3           |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 3        | 1.3           |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 3        | 1.3           |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 1        | 1.3           |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 1        | 1.3           |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 1        | 1.3           |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD12 | 1        | 1.3           |
| (1,257)  | 1:99:A:LEU:HD11  | 1:112:A:LYS:HG3  | 7        | 1.3           |
| (1,257)  | 1:99:A:LEU:HD12  | 1:112:A:LYS:HG3  | 7        | 1.3           |
| (1,257)  | 1:99:A:LEU:HD13  | 1:112:A:LYS:HG3  | 7        | 1.3           |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 1        | 1.29          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 1        | 1.29          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 1        | 1.29          |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 5        | 1.29          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 5        | 1.29          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 5        | 1.29          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 1        | 1.28          |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 2        | 1.28          |
| (1,17)   | 1:93:A:ASP:HA    | 1:169:A:MET:HG2  | 7        | 1.28          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 5        | 1.27          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3  | 9        | 1.27          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 5        | 1.27          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 9        | 1.27          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD1  | 1        | 1.27          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD2  | 1        | 1.27          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 8        | 1.26          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 3        | 1.26          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD1  | 3        | 1.26          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD2  | 3        | 1.26          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 1        | 1.26          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 4        | 1.26          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 9        | 1.25          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 3        | 1.25          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 8        | 1.25          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 10       | 1.25          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 10       | 1.25          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 10       | 1.25          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 10       | 1.25          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 10       | 1.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 10       | 1.25          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD1  | 7        | 1.25          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD2  | 7        | 1.25          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 2        | 1.25          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 4        | 1.25          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 4        | 1.25          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 7        | 1.24          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 5        | 1.24          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 10       | 1.24          |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 10       | 1.24          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 10       | 1.24          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 10       | 1.24          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 10       | 1.24          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 10       | 1.24          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 10       | 1.24          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 1        | 1.24          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 1        | 1.24          |
| (1,724)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB3  | 7        | 1.24          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 9        | 1.23          |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 9        | 1.23          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 9        | 1.23          |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 6        | 1.23          |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 9        | 1.23          |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 2        | 1.23          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE1  | 10       | 1.23          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE2  | 10       | 1.23          |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD12 | 5        | 1.23          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 6        | 1.23          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 7        | 1.22          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 7        | 1.22          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 7        | 1.22          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 2        | 1.22          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 2        | 1.22          |
| (1,4267) | 1:167:B:ALA:H    | 1:169:B:MET:H    | 2        | 1.21          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 6        | 1.21          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 10       | 1.21          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 10       | 1.21          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 10       | 1.21          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 6        | 1.21          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 4        | 1.21          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 4        | 1.21          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 4        | 1.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 6        | 1.21          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 6        | 1.21          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 6        | 1.21          |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD11 | 9        | 1.21          |
| (1,4)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB3   | 9        | 1.21          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 2        | 1.2           |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 3        | 1.2           |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 5        | 1.2           |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 2        | 1.2           |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 2        | 1.2           |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 2        | 1.2           |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 2        | 1.2           |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 2        | 1.2           |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 9        | 1.2           |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 7        | 1.2           |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 7        | 1.2           |
| (1,2004) | 1:171:A:LYS:H    | 1:169:A:MET:HA   | 9        | 1.2           |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 8        | 1.2           |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 8        | 1.2           |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 2        | 1.2           |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE1  | 1        | 1.2           |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE2  | 1        | 1.2           |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 6        | 1.19          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 7        | 1.19          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 8        | 1.19          |
| (1,2157) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 2        | 1.19          |
| (1,2025) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 2        | 1.19          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 6        | 1.19          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 6        | 1.19          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 6        | 1.19          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 5        | 1.19          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 2        | 1.19          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 2        | 1.19          |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 8        | 1.19          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 8        | 1.19          |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 8        | 1.19          |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 9        | 1.18          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 2        | 1.18          |
| (1,724)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB3  | 9        | 1.18          |
| (1,3)    | 1:89:A:ARG:HB2   | 1:90:A:HIS:HB2   | 6        | 1.18          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 1        | 1.17          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 1        | 1.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2 | 1        | 1.17          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2 | 5        | 1.17          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2 | 5        | 1.17          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2 | 5        | 1.17          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3 | 5        | 1.17          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3 | 5        | 1.17          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3 | 5        | 1.17          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2 | 1        | 1.17          |
| (1,2282) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HA   | 2        | 1.17          |
| (1,2282) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HA   | 2        | 1.17          |
| (1,2282) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HA   | 2        | 1.17          |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3 | 3        | 1.17          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3 | 3        | 1.17          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3 | 3        | 1.17          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2 | 6        | 1.16          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2 | 6        | 1.16          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2 | 6        | 1.16          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3 | 2        | 1.16          |
| (1,2391) | 1:96:B:ARG:HG3   | 1:166:B:GLU:HB3 | 6        | 1.16          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2 | 6        | 1.16          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3 | 7        | 1.16          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2 | 7        | 1.16          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2 | 7        | 1.16          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2 | 7        | 1.16          |
| (1,453)  | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3 | 9        | 1.16          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3 | 10       | 1.15          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3 | 10       | 1.15          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3 | 4        | 1.15          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3 | 4        | 1.15          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3 | 4        | 1.15          |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA  | 3        | 1.15          |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2 | 9        | 1.15          |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2 | 9        | 1.15          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2 | 2        | 1.15          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2 | 2        | 1.15          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2 | 2        | 1.15          |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2 | 1        | 1.14          |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2 | 7        | 1.14          |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2 | 7        | 1.14          |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2 | 7        | 1.14          |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2 | 1        | 1.14          |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2 | 7        | 1.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 7        | 1.14          |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 7        | 1.14          |
| (1,1614) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB2  | 7        | 1.14          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 9        | 1.14          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 3        | 1.14          |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD12 | 6        | 1.14          |
| (1,4283) | 1:169:B:MET:H    | 1:171:B:LYS:HE3  | 6        | 1.13          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 8        | 1.13          |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 6        | 1.13          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 9        | 1.13          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 9        | 1.13          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 9        | 1.13          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 3        | 1.13          |
| (1,2300) | 1:93:B:ASP:HB2   | 1:94:B:ARG:HG2   | 7        | 1.13          |
| (1,2003) | 1:171:A:LYS:H    | 1:92:A:ALA:HB1   | 3        | 1.13          |
| (1,2003) | 1:171:A:LYS:H    | 1:92:A:ALA:HB2   | 3        | 1.13          |
| (1,2003) | 1:171:A:LYS:H    | 1:92:A:ALA:HB3   | 3        | 1.13          |
| (1,1301) | 1:169:A:MET:HB3  | 1:171:A:LYS:HG2  | 9        | 1.13          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 5        | 1.13          |
| (1,17)   | 1:93:A:ASP:HA    | 1:169:A:MET:HG2  | 3        | 1.13          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 4        | 1.12          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 6        | 1.12          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 8        | 1.12          |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 7        | 1.12          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 7        | 1.12          |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 7        | 1.12          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 7        | 1.12          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 4        | 1.12          |
| (1,2194) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 3        | 1.12          |
| (1,2157) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 4        | 1.12          |
| (1,2062) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 3        | 1.12          |
| (1,2025) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 4        | 1.12          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 8        | 1.12          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 8        | 1.12          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 8        | 1.12          |
| (1,710)  | 1:126:A:GLU:HA   | 1:135:A:SER:HB2  | 2        | 1.12          |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 9        | 1.12          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 9        | 1.12          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 9        | 1.12          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD1  | 10       | 1.11          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD2  | 10       | 1.11          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 9        | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 9        | 1.11          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 9        | 1.11          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 10       | 1.11          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 10       | 1.11          |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 3        | 1.11          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 9        | 1.11          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 3        | 1.11          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 3        | 1.11          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 3        | 1.11          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 5        | 1.11          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 5        | 1.11          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 5        | 1.11          |
| (1,990)  | 1:148:A:VAL:HA   | 1:169:A:MET:HB2  | 3        | 1.11          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG21 | 7        | 1.11          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE1  | 3        | 1.11          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE2  | 3        | 1.11          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE1  | 3        | 1.11          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE2  | 3        | 1.11          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE1  | 3        | 1.11          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE2  | 3        | 1.11          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 9        | 1.1           |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 2        | 1.1           |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 2        | 1.1           |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 2        | 1.1           |
| (1,2284) | 1:89:B:ARG:HB2   | 1:90:B:HIS:HB2   | 6        | 1.1           |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 9        | 1.1           |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 6        | 1.1           |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 6        | 1.1           |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 6        | 1.1           |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 1        | 1.1           |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 1        | 1.1           |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 8        | 1.1           |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 9        | 1.1           |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 2        | 1.1           |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 2        | 1.1           |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 2        | 1.1           |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 10       | 1.1           |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 10       | 1.1           |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 10       | 1.1           |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 5        | 1.1           |
| (1,2)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HB3   | 2        | 1.1           |
| (1,2)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HB3   | 2        | 1.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HB3   | 2        | 1.1           |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 3        | 1.09          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 6        | 1.09          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 6        | 1.09          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 6        | 1.09          |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 4        | 1.09          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 6        | 1.09          |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 5        | 1.09          |
| (1,1269) | 1:167:A:ALA:HB1  | 1:168:A:PRO:HD2  | 9        | 1.09          |
| (1,1269) | 1:167:A:ALA:HB2  | 1:168:A:PRO:HD2  | 9        | 1.09          |
| (1,1269) | 1:167:A:ALA:HB3  | 1:168:A:PRO:HD2  | 9        | 1.09          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 8        | 1.09          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 8        | 1.09          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 8        | 1.09          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 7        | 1.09          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 8        | 1.09          |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 7        | 1.09          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 10       | 1.09          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 9        | 1.08          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 9        | 1.08          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 9        | 1.08          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 5        | 1.08          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 7        | 1.08          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 7        | 1.08          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 7        | 1.08          |
| (1,3346) | 1:152:B:GLN:HB2  | 1:169:B:MET:HA   | 6        | 1.08          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 5        | 1.08          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 5        | 1.08          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 7        | 1.08          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 6        | 1.08          |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 8        | 1.08          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 1        | 1.08          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 2        | 1.08          |
| (1,4267) | 1:167:B:ALA:H    | 1:169:B:MET:H    | 9        | 1.07          |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 4        | 1.07          |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 4        | 1.07          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 1        | 1.07          |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 3        | 1.07          |
| (1,17)   | 1:93:A:ASP:HA    | 1:169:A:MET:HG2  | 9        | 1.07          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 4        | 1.06          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 4        | 1.06          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 4        | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 5        | 1.06          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 5        | 1.06          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 5        | 1.06          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 2        | 1.06          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 2        | 1.06          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 2        | 1.06          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 3        | 1.06          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 3        | 1.06          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 3        | 1.06          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 3        | 1.06          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 3        | 1.06          |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 3        | 1.06          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 2        | 1.06          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 8        | 1.06          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 1        | 1.06          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 2        | 1.06          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG21  | 8        | 1.06          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG22  | 8        | 1.06          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG23  | 8        | 1.06          |
| (1,1301) | 1:169:A:MET:HB3  | 1:171:A:LYS:HG3  | 7        | 1.06          |
| (1,990)  | 1:148:A:VAL:HA   | 1:169:A:MET:HB2  | 4        | 1.06          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 3        | 1.06          |
| (1,918)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA3  | 8        | 1.06          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 9        | 1.06          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 3        | 1.05          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 3        | 1.05          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 3        | 1.05          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 8        | 1.05          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 4        | 1.05          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 4        | 1.05          |
| (1,722)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HA   | 7        | 1.05          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 7        | 1.05          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 7        | 1.05          |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 5        | 1.04          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 5        | 1.04          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 5        | 1.04          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 5        | 1.04          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 6        | 1.04          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 6        | 1.04          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 6        | 1.04          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 10       | 1.04          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 4        | 1.04          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 4        | 1.04          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 4        | 1.04          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 5        | 1.04          |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 5        | 1.04          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 5        | 1.04          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 7        | 1.04          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB1  | 8        | 1.04          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB2  | 8        | 1.04          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB3  | 8        | 1.04          |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB1  | 1        | 1.04          |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB2  | 1        | 1.04          |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB3  | 1        | 1.04          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 4        | 1.04          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 8        | 1.04          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 8        | 1.04          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 8        | 1.04          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE1  | 3        | 1.04          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE2  | 3        | 1.04          |
| (1,4076) | 1:152:B:GLN:H    | 1:170:B:PRO:HD2  | 1        | 1.03          |
| (1,3557) | 1:168:B:PRO:HA   | 1:169:B:MET:HG2  | 7        | 1.03          |
| (1,3199) | 1:144:B:LEU:HB3  | 1:147:B:GLY:HA3  | 9        | 1.03          |
| (1,2285) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB3   | 1        | 1.03          |
| (1,1302) | 1:169:A:MET:HB2  | 1:171:A:LYS:HE2  | 3        | 1.03          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 2        | 1.03          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 2        | 1.03          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 2        | 1.03          |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 1        | 1.03          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 1        | 1.03          |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 1        | 1.03          |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 5        | 1.03          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB1  | 1        | 1.03          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB2  | 1        | 1.03          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB3  | 1        | 1.03          |
| (1,16)   | 1:93:A:ASP:HA    | 1:94:A:ARG:HD2   | 8        | 1.03          |
| (1,7)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HA    | 9        | 1.03          |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 1        | 1.02          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 2        | 1.02          |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 2        | 1.02          |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 2        | 1.02          |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 2        | 1.02          |
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 2        | 1.02          |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 2        | 1.02          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 5        | 1.02          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 5        | 1.02          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 5        | 1.02          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 10       | 1.02          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 10       | 1.02          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 10       | 1.02          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 4        | 1.02          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 4        | 1.02          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 4        | 1.02          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 7        | 1.02          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 7        | 1.02          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 6        | 1.02          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 6        | 1.02          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 3        | 1.02          |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 4        | 1.01          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 8        | 1.01          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 8        | 1.01          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 8        | 1.01          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 1        | 1.01          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 1        | 1.01          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 5        | 1.01          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 1        | 1.01          |
| (1,2318) | 1:94:B:ARG:HB2   | 1:96:B:ARG:HA    | 7        | 1.01          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG21  | 5        | 1.01          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG22  | 5        | 1.01          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG23  | 5        | 1.01          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 7        | 1.01          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE1  | 5        | 1.01          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE2  | 5        | 1.01          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE1  | 5        | 1.01          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE2  | 5        | 1.01          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE1  | 5        | 1.01          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE2  | 5        | 1.01          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 2        | 1.0           |
| (1,3558) | 1:168:B:PRO:HA   | 1:169:B:MET:HG3  | 7        | 1.0           |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 1        | 1.0           |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 1        | 1.0           |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 1        | 1.0           |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 8        | 1.0           |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 7        | 1.0           |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 7        | 1.0           |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 7        | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 1        | 1.0           |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 1        | 1.0           |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 1        | 1.0           |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 1        | 1.0           |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 1        | 1.0           |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 1        | 1.0           |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 8        | 1.0           |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 8        | 1.0           |
| (1,4)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB3   | 2        | 1.0           |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 10       | 0.99          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 9        | 0.99          |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 5        | 0.99          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 10       | 0.99          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 10       | 0.99          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 10       | 0.99          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG21 | 9        | 0.99          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 5        | 0.99          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 9        | 0.99          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 9        | 0.99          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 9        | 0.99          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG21 | 3        | 0.99          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG22 | 3        | 0.99          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG23 | 3        | 0.99          |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG21  | 6        | 0.99          |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG22  | 6        | 0.99          |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG23  | 6        | 0.99          |
| (1,2283) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HB3   | 4        | 0.99          |
| (1,2283) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HB3   | 4        | 0.99          |
| (1,2283) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HB3   | 4        | 0.99          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 7        | 0.99          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 7        | 0.99          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 7        | 0.99          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 10       | 0.99          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 10       | 0.99          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 4        | 0.99          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 7        | 0.99          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB1  | 4        | 0.99          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB2  | 4        | 0.99          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB3  | 4        | 0.99          |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 8        | 0.98          |
| (1,3271) | 1:148:B:VAL:HA   | 1:169:B:MET:HB2  | 5        | 0.98          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 3        | 0.98          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 4        | 0.98          |
| (1,2352) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB2  | 7        | 0.98          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 7        | 0.98          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 7        | 0.98          |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 3        | 0.98          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD1  | 8        | 0.98          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD2  | 8        | 0.98          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 8        | 0.98          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE1  | 2        | 0.98          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE2  | 2        | 0.98          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE1  | 2        | 0.98          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE2  | 2        | 0.98          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE1  | 2        | 0.98          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE2  | 2        | 0.98          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 8        | 0.98          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 8        | 0.98          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 8        | 0.98          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB1  | 9        | 0.98          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB2  | 9        | 0.98          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB3  | 9        | 0.98          |
| (1,4293) | 1:172:B:LEU:H    | 1:171:B:LYS:HA   | 9        | 0.97          |
| (1,4283) | 1:169:B:MET:H    | 1:171:B:LYS:HE2  | 3        | 0.97          |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 1        | 0.97          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 1        | 0.97          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG2  | 3        | 0.97          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 9        | 0.97          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 10       | 0.97          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 10       | 0.97          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 10       | 0.97          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 3        | 0.97          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 3        | 0.97          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 3        | 0.97          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 6        | 0.97          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 6        | 0.97          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 6        | 0.97          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 6        | 0.97          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 6        | 0.97          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 9        | 0.97          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 9        | 0.97          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 9        | 0.97          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 9        | 0.97          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 9        | 0.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 9        | 0.97          |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 5        | 0.97          |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 5        | 0.97          |
| (1,2012) | 1:172:A:LEU:H    | 1:171:A:LYS:HA   | 8        | 0.97          |
| (1,1012) | 1:148:A:VAL:HG11 | 1:169:A:MET:HB2  | 4        | 0.97          |
| (1,1012) | 1:148:A:VAL:HG12 | 1:169:A:MET:HB2  | 4        | 0.97          |
| (1,1012) | 1:148:A:VAL:HG13 | 1:169:A:MET:HB2  | 4        | 0.97          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 8        | 0.97          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE1  | 7        | 0.97          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE2  | 7        | 0.97          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE1  | 7        | 0.97          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE2  | 7        | 0.97          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE1  | 7        | 0.97          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE2  | 7        | 0.97          |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 9        | 0.96          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 3        | 0.96          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 5        | 0.96          |
| (1,3550) | 1:167:B:ALA:HB1  | 1:168:B:PRO:HD2  | 3        | 0.96          |
| (1,3550) | 1:167:B:ALA:HB2  | 1:168:B:PRO:HD2  | 3        | 0.96          |
| (1,3550) | 1:167:B:ALA:HB3  | 1:168:B:PRO:HD2  | 3        | 0.96          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 8        | 0.96          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 8        | 0.96          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 8        | 0.96          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 9        | 0.96          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 9        | 0.96          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 9        | 0.96          |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 9        | 0.96          |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 10       | 0.96          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 6        | 0.96          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 6        | 0.96          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 6        | 0.96          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 1        | 0.96          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 1        | 0.96          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 1        | 0.96          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 7        | 0.96          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 7        | 0.96          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 7        | 0.96          |
| (1,453)  | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 3        | 0.96          |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 8        | 0.96          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 8        | 0.96          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 8        | 0.96          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 10       | 0.96          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB1  | 6        | 0.96          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB2  | 6        | 0.96          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB3  | 6        | 0.96          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 1        | 0.95          |
| (1,4255) | 1:167:B:ALA:H    | 1:95:B:TRP:HB3   | 8        | 0.95          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 2        | 0.95          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 2        | 0.95          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 2        | 0.95          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 2        | 0.95          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 7        | 0.95          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 10       | 0.95          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 3        | 0.95          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 3        | 0.95          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 3        | 0.95          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 4        | 0.95          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 8        | 0.95          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 2        | 0.95          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 2        | 0.95          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 2        | 0.95          |
| (1,1012) | 1:148:A:VAL:HG11 | 1:169:A:MET:HB2  | 3        | 0.95          |
| (1,1012) | 1:148:A:VAL:HG12 | 1:169:A:MET:HB2  | 3        | 0.95          |
| (1,1012) | 1:148:A:VAL:HG13 | 1:169:A:MET:HB2  | 3        | 0.95          |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 2        | 0.95          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB1  | 10       | 0.95          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB2  | 10       | 0.95          |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB3  | 10       | 0.95          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 8        | 0.94          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 8        | 0.94          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 8        | 0.94          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 6        | 0.94          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 7        | 0.94          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 4        | 0.94          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 4        | 0.94          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 4        | 0.94          |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 9        | 0.94          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 5        | 0.94          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 5        | 0.94          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 5        | 0.94          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 3        | 0.94          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 3        | 0.94          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 5        | 0.93          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 10       | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD12 | 9        | 0.93          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 2        | 0.93          |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 4        | 0.93          |
| (1,990)  | 1:148:A:VAL:HA   | 1:169:A:MET:HB2  | 10       | 0.93          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 6        | 0.93          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 6        | 0.93          |
| (1,724)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB3  | 6        | 0.93          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG23 | 3        | 0.93          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 1        | 0.93          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 3        | 0.92          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 1        | 0.92          |
| (1,3274) | 1:148:B:VAL:HA   | 1:170:B:PRO:HG2  | 2        | 0.92          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 3        | 0.92          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 3        | 0.92          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 3        | 0.92          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 5        | 0.92          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 4        | 0.92          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 8        | 0.92          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 8        | 0.92          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 8        | 0.92          |
| (1,2194) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 4        | 0.92          |
| (1,2062) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 4        | 0.92          |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 4        | 0.92          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 9        | 0.92          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 9        | 0.92          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 9        | 0.92          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 1        | 0.92          |
| (1,474)  | 1:112:A:LYS:HE3  | 1:114:A:LYS:HB3  | 1        | 0.92          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 5        | 0.92          |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 10       | 0.91          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 4        | 0.91          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 4        | 0.91          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 4        | 0.91          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1  | 4        | 0.91          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2  | 4        | 0.91          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 2        | 0.91          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 7        | 0.91          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 7        | 0.91          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 7        | 0.91          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 7        | 0.91          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 7        | 0.91          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 7        | 0.91          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2298) | 1:93:B:ASP:HA    | 1:169:B:MET:HG2 | 1        | 0.91          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3 | 3        | 0.91          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3 | 3        | 0.91          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3 | 3        | 0.91          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3 | 3        | 0.91          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3 | 5        | 0.91          |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2 | 7        | 0.91          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2 | 7        | 0.91          |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2 | 7        | 0.91          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA  | 4        | 0.91          |
| (1,4267) | 1:167:B:ALA:H    | 1:169:B:MET:H   | 10       | 0.9           |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3 | 6        | 0.9           |
| (1,3303) | 1:148:B:VAL:HG21 | 1:170:B:PRO:HG2 | 2        | 0.9           |
| (1,3303) | 1:148:B:VAL:HG22 | 1:170:B:PRO:HG2 | 2        | 0.9           |
| (1,3303) | 1:148:B:VAL:HG23 | 1:170:B:PRO:HG2 | 2        | 0.9           |
| (1,2976) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB2 | 10       | 0.9           |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1 | 8        | 0.9           |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2 | 8        | 0.9           |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3 | 7        | 0.9           |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2 | 8        | 0.9           |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2 | 8        | 0.9           |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2 | 8        | 0.9           |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA   | 5        | 0.9           |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2 | 5        | 0.9           |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2 | 5        | 0.9           |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2 | 5        | 0.9           |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2 | 5        | 0.9           |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2 | 5        | 0.9           |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2 | 5        | 0.9           |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG  | 8        | 0.9           |
| (1,2009) | 1:171:A:LYS:H    | 1:171:A:LYS:HB2 | 10       | 0.9           |
| (1,1916) | 1:162:A:THR:H    | 1:102:A:ASN:HB3 | 6        | 0.9           |
| (1,1916) | 1:162:A:THR:H    | 1:102:A:ASN:HB3 | 9        | 0.9           |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3 | 1        | 0.9           |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3 | 7        | 0.9           |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE1 | 10       | 0.9           |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE2 | 10       | 0.9           |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE1 | 10       | 0.9           |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE2 | 10       | 0.9           |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE1 | 10       | 0.9           |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE2 | 10       | 0.9           |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2 | 4        | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 8        | 0.9           |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB1  | 2        | 0.9           |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB2  | 2        | 0.9           |
| (1,63)   | 1:95:A:TRP:HB2   | 1:167:A:ALA:HB3  | 2        | 0.9           |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 4        | 0.89          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 1        | 0.89          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 10       | 0.89          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 10       | 0.89          |
| (1,1301) | 1:169:A:MET:HB3  | 1:171:A:LYS:HG2  | 3        | 0.89          |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 10       | 0.89          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 7        | 0.89          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 7        | 0.89          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 7        | 0.89          |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 2        | 0.89          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 2        | 0.89          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 2        | 0.89          |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 10       | 0.89          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 10       | 0.89          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 10       | 0.89          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 7        | 0.89          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 7        | 0.89          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 7        | 0.89          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 4        | 0.89          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 4        | 0.89          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 4        | 0.89          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 10       | 0.89          |
| (1,4086) | 1:152:B:GLN:HE21 | 1:170:B:PRO:HD3  | 3        | 0.88          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 7        | 0.88          |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 6        | 0.88          |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 4        | 0.88          |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 6        | 0.88          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 5        | 0.88          |
| (1,1018) | 1:148:A:VAL:HG21 | 1:168:A:PRO:HD3  | 10       | 0.88          |
| (1,1018) | 1:148:A:VAL:HG22 | 1:168:A:PRO:HD3  | 10       | 0.88          |
| (1,1018) | 1:148:A:VAL:HG23 | 1:168:A:PRO:HD3  | 10       | 0.88          |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD3  | 4        | 0.87          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG22 | 7        | 0.87          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 4        | 0.87          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 4        | 0.87          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 4        | 0.87          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 10       | 0.87          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 10       | 0.87          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1 | 10       | 0.87          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2 | 10       | 0.87          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1 | 10       | 0.87          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2 | 10       | 0.87          |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2  | 9        | 0.87          |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA   | 4        | 0.87          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2 | 7        | 0.87          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2 | 7        | 0.87          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2 | 7        | 0.87          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2 | 7        | 0.87          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2 | 7        | 0.87          |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2 | 7        | 0.87          |
| (1,2004) | 1:171:A:LYS:H    | 1:169:A:MET:HA  | 2        | 0.87          |
| (1,2004) | 1:171:A:LYS:H    | 1:169:A:MET:HA  | 8        | 0.87          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1 | 9        | 0.87          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2 | 9        | 0.87          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3 | 9        | 0.87          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1 | 10       | 0.87          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2 | 10       | 0.87          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE1 | 9        | 0.87          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE2 | 9        | 0.87          |
| (1,704)  | 1:125:A:GLU:HA   | 1:135:A:SER:HB3 | 3        | 0.87          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE1 | 5        | 0.87          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE2 | 5        | 0.87          |
| (1,453)  | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3 | 7        | 0.87          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3 | 10       | 0.87          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3 | 10       | 0.87          |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3 | 10       | 0.87          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE1 | 6        | 0.87          |
| (1,254)  | 1:99:A:LEU:HD21  | 1:142:A:TYR:HE2 | 6        | 0.87          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE1 | 6        | 0.87          |
| (1,254)  | 1:99:A:LEU:HD22  | 1:142:A:TYR:HE2 | 6        | 0.87          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE1 | 6        | 0.87          |
| (1,254)  | 1:99:A:LEU:HD23  | 1:142:A:TYR:HE2 | 6        | 0.87          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2 | 1        | 0.87          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2 | 4        | 0.87          |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2 | 8        | 0.87          |
| (1,3763) | 1:114:B:LYS:H    | 1:115:B:ASP:HB2 | 2        | 0.86          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1 | 8        | 0.86          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2 | 8        | 0.86          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2 | 9        | 0.86          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2 | 10       | 0.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 4        | 0.86          |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 5        | 0.86          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 8        | 0.86          |
| (1,1012) | 1:148:A:VAL:HG11 | 1:169:A:MET:HB2  | 10       | 0.86          |
| (1,1012) | 1:148:A:VAL:HG12 | 1:169:A:MET:HB2  | 10       | 0.86          |
| (1,1012) | 1:148:A:VAL:HG13 | 1:169:A:MET:HB2  | 10       | 0.86          |
| (1,684)  | 1:123:A:LYS:HA   | 1:135:A:SER:HB3  | 5        | 0.86          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 2        | 0.86          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 6        | 0.86          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 7        | 0.86          |
| (1,4293) | 1:172:B:LEU:H    | 1:171:B:LYS:HA   | 3        | 0.85          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 1        | 0.85          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 1        | 0.85          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 1        | 0.85          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 5        | 0.85          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 10       | 0.85          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 10       | 0.85          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 10       | 0.85          |
| (1,2567) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB2  | 5        | 0.85          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 5        | 0.85          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 5        | 0.85          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 10       | 0.85          |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 6        | 0.85          |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 5        | 0.85          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 6        | 0.85          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 6        | 0.85          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 6        | 0.85          |
| (1,453)  | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 6        | 0.85          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 7        | 0.85          |
| (1,4076) | 1:152:B:GLN:H    | 1:170:B:PRO:HD3  | 3        | 0.84          |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 10       | 0.84          |
| (1,3293) | 1:148:B:VAL:HG11 | 1:169:B:MET:HB2  | 5        | 0.84          |
| (1,3293) | 1:148:B:VAL:HG12 | 1:169:B:MET:HB2  | 5        | 0.84          |
| (1,3293) | 1:148:B:VAL:HG13 | 1:169:B:MET:HB2  | 5        | 0.84          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 9        | 0.84          |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 3        | 0.84          |
| (1,2298) | 1:93:B:ASP:HA    | 1:169:B:MET:HG2  | 8        | 0.84          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 9        | 0.84          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 9        | 0.84          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE1  | 6        | 0.84          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE2  | 6        | 0.84          |
| (1,728)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HA   | 2        | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 7        | 0.84          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 7        | 0.84          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 7        | 0.84          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 4        | 0.84          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 4        | 0.84          |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 4        | 0.84          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 5        | 0.84          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 9        | 0.84          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 9        | 0.84          |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 1        | 0.84          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 7        | 0.83          |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 8        | 0.83          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 7        | 0.83          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 7        | 0.83          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 7        | 0.83          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 6        | 0.83          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 6        | 0.83          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 9        | 0.83          |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 4        | 0.83          |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 2        | 0.83          |
| (1,2353) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB3  | 7        | 0.83          |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 7        | 0.83          |
| (1,2290) | 1:90:B:HIS:HB3   | 1:91:B:THR:HA    | 5        | 0.83          |
| (1,2012) | 1:172:A:LEU:H    | 1:171:A:LYS:HA   | 10       | 0.83          |
| (1,1998) | 1:169:A:MET:H    | 1:169:A:MET:HB2  | 3        | 0.83          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 4        | 0.83          |
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 2        | 0.83          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 4        | 0.83          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 4        | 0.83          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 4        | 0.83          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 5        | 0.83          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 5        | 0.83          |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 5        | 0.83          |
| (1,7)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HA    | 1        | 0.83          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 5        | 0.83          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 8        | 0.82          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 4        | 0.82          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG11 | 10       | 0.82          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG12 | 10       | 0.82          |
| (1,3408) | 1:155:B:SER:HB3  | 1:165:B:VAL:HG13 | 10       | 0.82          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 8        | 0.82          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 7        | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 7        | 0.82          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 7        | 0.82          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 8        | 0.82          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 8        | 0.82          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 8        | 0.82          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 2        | 0.82          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1  | 7        | 0.82          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2  | 7        | 0.82          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 2        | 0.82          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD3   | 7        | 0.82          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 8        | 0.82          |
| (1,827)  | 1:139:A:THR:HA   | 1:140:A:ARG:HG2  | 3        | 0.82          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE1  | 2        | 0.82          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE2  | 2        | 0.82          |
| (1,728)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HA   | 5        | 0.82          |
| (1,722)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HA   | 5        | 0.82          |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 1        | 0.82          |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 1        | 0.82          |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 1        | 0.82          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 3        | 0.82          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 6        | 0.82          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 3        | 0.82          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 3        | 0.82          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 3        | 0.82          |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 6        | 0.82          |
| (1,1)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HA    | 7        | 0.82          |
| (1,1)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HA    | 7        | 0.82          |
| (1,1)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HA    | 7        | 0.82          |
| (1,4280) | 1:169:B:MET:H    | 1:169:B:MET:HB3  | 7        | 0.81          |
| (1,4272) | 1:169:B:MET:H    | 1:95:B:TRP:HA    | 6        | 0.81          |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 5        | 0.81          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 2        | 0.81          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 2        | 0.81          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 2        | 0.81          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 7        | 0.81          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 7        | 0.81          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 7        | 0.81          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 10       | 0.81          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 10       | 0.81          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 10       | 0.81          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 4        | 0.81          |
| (1,2991) | 1:126:B:GLU:HA   | 1:135:B:SER:HB2  | 4        | 0.81          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 9        | 0.81          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1  | 1        | 0.81          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2  | 1        | 0.81          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG21 | 8        | 0.81          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG22 | 8        | 0.81          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG23 | 8        | 0.81          |
| (1,2285) | 1:89:B:ARG:HB2   | 1:90:B:HIS:HB3   | 10       | 0.81          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 9        | 0.81          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 9        | 0.81          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 9        | 0.81          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 9        | 0.81          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 9        | 0.81          |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 9        | 0.81          |
| (1,1998) | 1:169:A:MET:H    | 1:169:A:MET:HB2  | 4        | 0.81          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 4        | 0.81          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 10       | 0.81          |
| (1,1482) | 1:114:A:LYS:H    | 1:115:A:ASP:HB2  | 5        | 0.81          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 2        | 0.81          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG22 | 6        | 0.81          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 1        | 0.81          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 1        | 0.81          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 1        | 0.81          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 2        | 0.81          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 5        | 0.81          |
| (1,4288) | 1:171:B:LYS:H    | 1:170:B:PRO:HD3  | 5        | 0.8           |
| (1,4197) | 1:162:B:THR:H    | 1:102:B:ASN:HB3  | 10       | 0.8           |
| (1,4095) | 1:152:B:GLN:HE22 | 1:170:B:PRO:HD3  | 2        | 0.8           |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 5        | 0.8           |
| (1,3763) | 1:114:B:LYS:H    | 1:115:B:ASP:HB2  | 6        | 0.8           |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 3        | 0.8           |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 4        | 0.8           |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 4        | 0.8           |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 4        | 0.8           |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 10       | 0.8           |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 10       | 0.8           |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 10       | 0.8           |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 8        | 0.8           |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 8        | 0.8           |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 8        | 0.8           |
| (1,2976) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB2  | 4        | 0.8           |
| (1,2538) | 1:99:B:LEU:HD21  | 1:112:B:LYS:HG3  | 3        | 0.8           |
| (1,2538) | 1:99:B:LEU:HD22  | 1:112:B:LYS:HG3  | 3        | 0.8           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2538) | 1:99:B:LEU:HD23  | 1:112:B:LYS:HG3  | 3        | 0.8           |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 10       | 0.8           |
| (1,2281) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 10       | 0.8           |
| (1,2148) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 10       | 0.8           |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 1        | 0.8           |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 1        | 0.8           |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 1        | 0.8           |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 1        | 0.8           |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 1        | 0.8           |
| (1,688)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB3  | 3        | 0.8           |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG21  | 10       | 0.8           |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG22  | 10       | 0.8           |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG23  | 10       | 0.8           |
| (1,2)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HB3   | 1        | 0.8           |
| (1,2)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HB3   | 1        | 0.8           |
| (1,2)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HB3   | 1        | 0.8           |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 3        | 0.79          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 9        | 0.79          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 9        | 0.79          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 9        | 0.79          |
| (1,3346) | 1:152:B:GLN:HB2  | 1:169:B:MET:HA   | 4        | 0.79          |
| (1,3345) | 1:152:B:GLN:HB2  | 1:168:B:PRO:HD3  | 3        | 0.79          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 4        | 0.79          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 10       | 0.79          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 8        | 0.79          |
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 6        | 0.79          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 6        | 0.79          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 6        | 0.79          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 6        | 0.79          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 2        | 0.79          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 2        | 0.79          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 2        | 0.79          |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 1        | 0.79          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 6        | 0.79          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 6        | 0.79          |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 2        | 0.79          |
| (1,2009) | 1:171:A:LYS:H    | 1:171:A:LYS:HB3  | 5        | 0.79          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 7        | 0.79          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 7        | 0.79          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 7        | 0.79          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 7        | 0.79          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 9        | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 8        | 0.79          |
| (1,71)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB2  | 10       | 0.79          |
| (1,1)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HA    | 6        | 0.79          |
| (1,1)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HA    | 6        | 0.79          |
| (1,1)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HA    | 6        | 0.79          |
| (1,4065) | 1:152:B:GLN:H    | 1:149:B:ASP:HB3  | 5        | 0.78          |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 8        | 0.78          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 10       | 0.78          |
| (1,3895) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB2  | 10       | 0.78          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 2        | 0.78          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 2        | 0.78          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 2        | 0.78          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 2        | 0.78          |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 3        | 0.78          |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 10       | 0.78          |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 3        | 0.78          |
| (1,2007) | 1:171:A:LYS:H    | 1:170:A:PRO:HD3  | 9        | 0.78          |
| (1,1799) | 1:152:A:GLN:HE21 | 1:152:A:GLN:HB3  | 6        | 0.78          |
| (1,1691) | 1:140:A:ARG:H    | 1:120:A:ILE:HB   | 9        | 0.78          |
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 10       | 0.78          |
| (1,827)  | 1:139:A:THR:HA   | 1:140:A:ARG:HG2  | 4        | 0.78          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG23 | 4        | 0.78          |
| (1,684)  | 1:123:A:LYS:HA   | 1:135:A:SER:HB3  | 2        | 0.78          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 9        | 0.78          |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 10       | 0.78          |
| (1,4255) | 1:167:B:ALA:H    | 1:95:B:TRP:HB3   | 4        | 0.77          |
| (1,4080) | 1:152:B:GLN:HE21 | 1:152:B:GLN:HB3  | 3        | 0.77          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 1        | 0.77          |
| (1,3346) | 1:152:B:GLN:HB2  | 1:169:B:MET:HA   | 9        | 0.77          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG23 | 1        | 0.77          |
| (1,2976) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HB2  | 3        | 0.77          |
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 5        | 0.77          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 7        | 0.77          |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 10       | 0.77          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 6        | 0.77          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 6        | 0.77          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 6        | 0.77          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 6        | 0.77          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 6        | 0.77          |
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 6        | 0.77          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 4        | 0.77          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 6        | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,990)  | 1:148:A:VAL:HA   | 1:169:A:MET:HB2  | 5        | 0.77          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 4        | 0.77          |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG23 | 4        | 0.77          |
| (1,710)  | 1:126:A:GLU:HA   | 1:135:A:SER:HB2  | 7        | 0.77          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 10       | 0.77          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 4        | 0.77          |
| (1,4272) | 1:169:B:MET:H    | 1:95:B:TRP:HA    | 5        | 0.76          |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 7        | 0.76          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 10       | 0.76          |
| (1,3271) | 1:148:B:VAL:HA   | 1:169:B:MET:HB2  | 4        | 0.76          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 1        | 0.76          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 1        | 0.76          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 1        | 0.76          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 7        | 0.76          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 7        | 0.76          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 7        | 0.76          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 7        | 0.76          |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 5        | 0.76          |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 5        | 0.76          |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 5        | 0.76          |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 5        | 0.76          |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 5        | 0.76          |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 5        | 0.76          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 2        | 0.76          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 5        | 0.76          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 3        | 0.76          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 5        | 0.76          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 3        | 0.76          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 4        | 0.76          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 8        | 0.76          |
| (1,731)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 8        | 0.76          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 5        | 0.76          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 4        | 0.76          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 4        | 0.76          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 4        | 0.76          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 10       | 0.76          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 10       | 0.76          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 10       | 0.76          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 10       | 0.76          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 10       | 0.76          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 10       | 0.76          |
| (1,99)   | 1:96:A:ARG:HB3   | 1:164:A:THR:HB   | 7        | 0.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 10       | 0.76          |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG2  | 10       | 0.75          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 5        | 0.75          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 5        | 0.75          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 5        | 0.75          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 5        | 0.75          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 5        | 0.75          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 5        | 0.75          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 1        | 0.75          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 1        | 0.75          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 1        | 0.75          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 1        | 0.75          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 3        | 0.75          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 7        | 0.75          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 7        | 0.75          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 7        | 0.75          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG21 | 10       | 0.75          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG22 | 10       | 0.75          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG23 | 10       | 0.75          |
| (1,2284) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB2   | 1        | 0.75          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 3        | 0.75          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 3        | 0.75          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 3        | 0.75          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 6        | 0.75          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 6        | 0.75          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 6        | 0.75          |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 3        | 0.75          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 6        | 0.75          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 9        | 0.75          |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB1  | 3        | 0.74          |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB2  | 3        | 0.74          |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB3  | 3        | 0.74          |
| (1,4076) | 1:152:B:GLN:H    | 1:170:B:PRO:HD2  | 2        | 0.74          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 4        | 0.74          |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 9        | 0.74          |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 9        | 0.74          |
| (1,2976) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB2  | 1        | 0.74          |
| (1,2151) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 8        | 0.74          |
| (1,2151) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 8        | 0.74          |
| (1,2151) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 8        | 0.74          |
| (1,2019) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB2  | 8        | 0.74          |
| (1,2019) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB2  | 8        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2019) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB2  | 8        | 0.74          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 3        | 0.74          |
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 2        | 0.74          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 3        | 0.74          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 3        | 0.74          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 3        | 0.74          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 10       | 0.74          |
| (1,385)  | 1:109:A:LEU:HD21 | 1:161:A:GLY:HA3  | 4        | 0.74          |
| (1,385)  | 1:109:A:LEU:HD22 | 1:161:A:GLY:HA3  | 4        | 0.74          |
| (1,385)  | 1:109:A:LEU:HD23 | 1:161:A:GLY:HA3  | 4        | 0.74          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 3        | 0.74          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 3        | 0.74          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 3        | 0.74          |
| (1,327)  | 1:106:A:PRO:HG3  | 1:157:A:LEU:HD12 | 3        | 0.74          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 1        | 0.74          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 1        | 0.74          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 1        | 0.74          |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 3        | 0.74          |
| (1,8)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HG21  | 4        | 0.74          |
| (1,8)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HG22  | 4        | 0.74          |
| (1,8)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HG23  | 4        | 0.74          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 6        | 0.73          |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 1        | 0.73          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 2        | 0.73          |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE2  | 10       | 0.73          |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE2  | 10       | 0.73          |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE2  | 10       | 0.73          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 4        | 0.73          |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 10       | 0.73          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 6        | 0.73          |
| (1,1608) | 1:128:A:GLN:HE22 | 1:128:A:GLN:HB2  | 7        | 0.73          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 4        | 0.73          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 4        | 0.73          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 4        | 0.73          |
| (1,715)  | 1:126:A:GLU:HB2  | 1:135:A:SER:HB3  | 6        | 0.73          |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 4        | 0.73          |
| (1,3)    | 1:89:A:ARG:HB3   | 1:90:A:HIS:HB2   | 3        | 0.73          |
| (1,1)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HA    | 9        | 0.73          |
| (1,1)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HA    | 9        | 0.73          |
| (1,1)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HA    | 9        | 0.73          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 6        | 0.72          |
| (1,4048) | 1:149:B:ASP:H    | 1:170:B:PRO:HG3  | 5        | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD1  | 3        | 0.72          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD2  | 3        | 0.72          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 1        | 0.72          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 9        | 0.72          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 5        | 0.72          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 5        | 0.72          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 5        | 0.72          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 3        | 0.72          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 3        | 0.72          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 3        | 0.72          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 8        | 0.72          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 8        | 0.72          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 8        | 0.72          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 5        | 0.72          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 5        | 0.72          |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 8        | 0.72          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG21 | 3        | 0.72          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG22 | 3        | 0.72          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG23 | 3        | 0.72          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 3        | 0.72          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 3        | 0.72          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 3        | 0.72          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 3        | 0.72          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 3        | 0.72          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 3        | 0.72          |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 3        | 0.72          |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 3        | 0.72          |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 3        | 0.72          |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 3        | 0.72          |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 3        | 0.72          |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 3        | 0.72          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 1        | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 1        | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 1        | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 1        | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 2        | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 2        | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 2        | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 10       | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 10       | 0.72          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 10       | 0.72          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG21 | 2        | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE1  | 2        | 0.72          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE2  | 2        | 0.72          |
| (1,405)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HD2  | 1        | 0.72          |
| (1,405)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HD2  | 1        | 0.72          |
| (1,405)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HD2  | 1        | 0.72          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 2        | 0.72          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 2        | 0.72          |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 2        | 0.72          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 9        | 0.72          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 8        | 0.72          |
| (1,4294) | 1:172:B:LEU:H    | 1:172:B:LEU:HB3  | 3        | 0.71          |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 10       | 0.71          |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 6        | 0.71          |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 10       | 0.71          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 8        | 0.71          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 8        | 0.71          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 8        | 0.71          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 9        | 0.71          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 7        | 0.71          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 9        | 0.71          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1  | 10       | 0.71          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2  | 10       | 0.71          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 1        | 0.71          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 1        | 0.71          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 1        | 0.71          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 4        | 0.71          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 4        | 0.71          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 4        | 0.71          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 4        | 0.71          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 4        | 0.71          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 4        | 0.71          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG21 | 7        | 0.71          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG22 | 7        | 0.71          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG23 | 7        | 0.71          |
| (1,2213) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 1        | 0.71          |
| (1,2213) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 5        | 0.71          |
| (1,2081) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 1        | 0.71          |
| (1,2081) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 5        | 0.71          |
| (1,2000) | 1:169:A:MET:H    | 1:169:A:MET:HG3  | 7        | 0.71          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 8        | 0.71          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 8        | 0.71          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 8        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 4        | 0.71          |
| (1,1012) | 1:148:A:VAL:HG11 | 1:169:A:MET:HB2  | 5        | 0.71          |
| (1,1012) | 1:148:A:VAL:HG12 | 1:169:A:MET:HB2  | 5        | 0.71          |
| (1,1012) | 1:148:A:VAL:HG13 | 1:169:A:MET:HB2  | 5        | 0.71          |
| (1,958)  | 1:145:A:PRO:HG3  | 1:146:A:PRO:HD2  | 10       | 0.71          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE1  | 9        | 0.71          |
| (1,763)  | 1:128:A:GLN:HG3  | 1:133:A:TYR:HE2  | 9        | 0.71          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 1        | 0.71          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 1        | 0.71          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 1        | 0.71          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 10       | 0.71          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 6        | 0.71          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 6        | 0.71          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 6        | 0.71          |
| (1,71)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB2  | 7        | 0.71          |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB1  | 1        | 0.7           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB2  | 1        | 0.7           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB3  | 1        | 0.7           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB1  | 9        | 0.7           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB2  | 9        | 0.7           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB3  | 9        | 0.7           |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 8        | 0.7           |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 5        | 0.7           |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 5        | 0.7           |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 7        | 0.7           |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 7        | 0.7           |
| (1,2988) | 1:126:B:GLU:HA   | 1:133:B:TYR:HB3  | 6        | 0.7           |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 1        | 0.7           |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 7        | 0.7           |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 2        | 0.7           |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 2        | 0.7           |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 2        | 0.7           |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 2        | 0.7           |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 2        | 0.7           |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 2        | 0.7           |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 4        | 0.7           |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 10       | 0.7           |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 10       | 0.7           |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 10       | 0.7           |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG22 | 1        | 0.7           |
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 3        | 0.7           |
| (1,958)  | 1:145:A:PRO:HG3  | 1:146:A:PRO:HD2  | 5        | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 4        | 0.7           |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 6        | 0.7           |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 9        | 0.7           |
| (1,9)    | 1:90:A:HIS:HB3   | 1:91:A:THR:HA    | 10       | 0.7           |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 1        | 0.7           |
| (1,4270) | 1:169:B:MET:H    | 1:94:B:ARG:HB3   | 6        | 0.69          |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 7        | 0.69          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 1        | 0.69          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 1        | 0.69          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 1        | 0.69          |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 2        | 0.69          |
| (1,3096) | 1:136:B:ARG:HG3  | 1:138:B:PHE:HA   | 10       | 0.69          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 1        | 0.69          |
| (1,2545) | 1:100:B:ASP:HB2  | 1:162:B:THR:HB   | 1        | 0.69          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 5        | 0.69          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 4        | 0.69          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 6        | 0.69          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 7        | 0.69          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 7        | 0.69          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 7        | 0.69          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG23 | 8        | 0.69          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 6        | 0.69          |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 5        | 0.69          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 5        | 0.69          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 5        | 0.69          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 1        | 0.69          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 9        | 0.69          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 8        | 0.68          |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 9        | 0.68          |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 4        | 0.68          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE1  | 1        | 0.68          |
| (1,3044) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HE2  | 1        | 0.68          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 5        | 0.68          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 5        | 0.68          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 5        | 0.68          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG21 | 9        | 0.68          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG22 | 9        | 0.68          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG23 | 9        | 0.68          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG21 | 10       | 0.68          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG22 | 10       | 0.68          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG23 | 10       | 0.68          |
| (1,2619) | 1:108:B:GLU:HA   | 1:123:B:LYS:HD2  | 1        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 5        | 0.68          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 5        | 0.68          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 5        | 0.68          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 6        | 0.68          |
| (1,2007) | 1:171:A:LYS:H    | 1:170:A:PRO:HD3  | 10       | 0.68          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 2        | 0.68          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 2        | 0.68          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 2        | 0.68          |
| (1,1691) | 1:140:A:ARG:H    | 1:120:A:ILE:HB   | 6        | 0.68          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 2        | 0.68          |
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 8        | 0.68          |
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 9        | 0.68          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 9        | 0.68          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 9        | 0.68          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 9        | 0.68          |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 4        | 0.68          |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 7        | 0.68          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 9        | 0.68          |
| (1,684)  | 1:123:A:LYS:HA   | 1:135:A:SER:HB3  | 3        | 0.68          |
| (1,232)  | 1:99:A:LEU:HD11  | 1:120:A:ILE:HG12 | 7        | 0.68          |
| (1,232)  | 1:99:A:LEU:HD12  | 1:120:A:ILE:HG12 | 7        | 0.68          |
| (1,232)  | 1:99:A:LEU:HD13  | 1:120:A:ILE:HG12 | 7        | 0.68          |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 7        | 0.68          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB1   | 6        | 0.67          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB2   | 6        | 0.67          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB3   | 6        | 0.67          |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 5        | 0.67          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 7        | 0.67          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 4        | 0.67          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 8        | 0.67          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 5        | 0.67          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 5        | 0.67          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 9        | 0.67          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 4        | 0.67          |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 1        | 0.67          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 5        | 0.67          |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 1        | 0.67          |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG21 | 2        | 0.67          |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG21 | 6        | 0.67          |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG23 | 8        | 0.67          |
| (1,1614) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB2  | 3        | 0.67          |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 1        | 0.67          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1413) | 1:108:A:GLU:H   | 1:106:A:PRO:HB3  | 5        | 0.67          |
| (1,1333) | 1:95:A:TRP:H    | 1:166:A:GLU:HG3  | 1        | 0.67          |
| (1,1163) | 1:157:A:LEU:HG  | 1:161:A:GLY:HA3  | 1        | 0.67          |
| (1,710)  | 1:126:A:GLU:HA  | 1:135:A:SER:HB2  | 9        | 0.67          |
| (1,695)  | 1:123:A:LYS:HD3 | 1:137:A:CYS:HB2  | 10       | 0.67          |
| (1,688)  | 1:123:A:LYS:HB2 | 1:137:A:CYS:HB3  | 5        | 0.67          |
| (1,232)  | 1:99:A:LEU:HD11 | 1:120:A:ILE:HG12 | 6        | 0.67          |
| (1,232)  | 1:99:A:LEU:HD12 | 1:120:A:ILE:HG12 | 6        | 0.67          |
| (1,232)  | 1:99:A:LEU:HD13 | 1:120:A:ILE:HG12 | 6        | 0.67          |
| (1,77)   | 1:95:A:TRP:HE3  | 1:167:A:ALA:HB1  | 9        | 0.67          |
| (1,77)   | 1:95:A:TRP:HE3  | 1:167:A:ALA:HB2  | 9        | 0.67          |
| (1,77)   | 1:95:A:TRP:HE3  | 1:167:A:ALA:HB3  | 9        | 0.67          |
| (1,63)   | 1:95:A:TRP:HB2  | 1:167:A:ALA:HB1  | 7        | 0.67          |
| (1,63)   | 1:95:A:TRP:HB2  | 1:167:A:ALA:HB2  | 7        | 0.67          |
| (1,63)   | 1:95:A:TRP:HB2  | 1:167:A:ALA:HB3  | 7        | 0.67          |
| (1,4)    | 1:89:A:ARG:HB3  | 1:90:A:HIS:HB3   | 5        | 0.67          |
| (1,3)    | 1:89:A:ARG:HB2  | 1:90:A:HIS:HB2   | 9        | 0.67          |
| (1,3694) | 1:108:B:GLU:H   | 1:106:B:PRO:HB3  | 7        | 0.66          |
| (1,3694) | 1:108:B:GLU:H   | 1:106:B:PRO:HB3  | 8        | 0.66          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD21 | 7        | 0.66          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD22 | 7        | 0.66          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD23 | 7        | 0.66          |
| (1,3193) | 1:144:B:LEU:HB2 | 1:148:B:VAL:HG11 | 5        | 0.66          |
| (1,3193) | 1:144:B:LEU:HB2 | 1:148:B:VAL:HG12 | 5        | 0.66          |
| (1,3193) | 1:144:B:LEU:HB2 | 1:148:B:VAL:HG13 | 5        | 0.66          |
| (1,3010) | 1:126:B:GLU:HG3 | 1:133:B:TYR:HB3  | 3        | 0.66          |
| (1,3009) | 1:126:B:GLU:HG3 | 1:133:B:TYR:HA   | 4        | 0.66          |
| (1,2986) | 1:126:B:GLU:HA  | 1:126:B:GLU:HG3  | 6        | 0.66          |
| (1,2755) | 1:112:B:LYS:HE2 | 1:114:B:LYS:HB3  | 8        | 0.66          |
| (1,2608) | 1:106:B:PRO:HG3 | 1:157:B:LEU:HD13 | 1        | 0.66          |
| (1,2385) | 1:96:B:ARG:HG2  | 1:166:B:GLU:HA   | 7        | 0.66          |
| (1,2314) | 1:94:B:ARG:HA   | 1:169:B:MET:HB2  | 2        | 0.66          |
| (1,2312) | 1:94:B:ARG:HA   | 1:168:B:PRO:HD2  | 6        | 0.66          |
| (1,2157) | 1:132:B:GLY:HA2 | 1:140:A:ARG:HA   | 10       | 0.66          |
| (1,2025) | 1:132:B:GLY:HA2 | 1:140:A:ARG:HA   | 10       | 0.66          |
| (1,2015) | 1:173:A:ALA:H   | 1:172:A:LEU:HG   | 7        | 0.66          |
| (1,1950) | 1:165:A:VAL:H   | 1:96:A:ARG:HB2   | 9        | 0.66          |
| (1,1920) | 1:162:A:THR:H   | 1:158:A:SER:HB2  | 4        | 0.66          |
| (1,1843) | 1:154:A:SER:H   | 1:167:A:ALA:HB1  | 4        | 0.66          |
| (1,1843) | 1:154:A:SER:H   | 1:167:A:ALA:HB2  | 4        | 0.66          |
| (1,1843) | 1:154:A:SER:H   | 1:167:A:ALA:HB3  | 4        | 0.66          |
| (1,1665) | 1:135:A:SER:H   | 1:134:A:ILE:HD11 | 4        | 0.66          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1665) | 1:135:A:SER:H   | 1:134:A:ILE:HG23 | 7        | 0.66          |
| (1,1597) | 1:128:A:GLN:H   | 1:127:A:ARG:HB3  | 5        | 0.66          |
| (1,1413) | 1:108:A:GLU:H   | 1:106:A:PRO:HB3  | 1        | 0.66          |
| (1,1413) | 1:108:A:GLU:H   | 1:106:A:PRO:HB3  | 6        | 0.66          |
| (1,1319) | 1:94:A:ARG:H    | 1:91:A:THR:HG21  | 4        | 0.66          |
| (1,1319) | 1:94:A:ARG:H    | 1:91:A:THR:HG22  | 4        | 0.66          |
| (1,1319) | 1:94:A:ARG:H    | 1:91:A:THR:HG23  | 4        | 0.66          |
| (1,1192) | 1:158:A:SER:HB2 | 1:162:A:THR:HB   | 9        | 0.66          |
| (1,1140) | 1:156:A:SER:HB3 | 1:157:A:LEU:HD21 | 7        | 0.66          |
| (1,1140) | 1:156:A:SER:HB3 | 1:157:A:LEU:HD22 | 7        | 0.66          |
| (1,1140) | 1:156:A:SER:HB3 | 1:157:A:LEU:HD23 | 7        | 0.66          |
| (1,1139) | 1:156:A:SER:HB3 | 1:157:A:LEU:HB3  | 2        | 0.66          |
| (1,1139) | 1:156:A:SER:HB3 | 1:157:A:LEU:HB3  | 10       | 0.66          |
| (1,958)  | 1:145:A:PRO:HG3 | 1:146:A:PRO:HD2  | 2        | 0.66          |
| (1,958)  | 1:145:A:PRO:HG3 | 1:146:A:PRO:HD2  | 3        | 0.66          |
| (1,958)  | 1:145:A:PRO:HG3 | 1:146:A:PRO:HD2  | 9        | 0.66          |
| (1,77)   | 1:95:A:TRP:HE3  | 1:167:A:ALA:HB1  | 6        | 0.66          |
| (1,77)   | 1:95:A:TRP:HE3  | 1:167:A:ALA:HB2  | 6        | 0.66          |
| (1,77)   | 1:95:A:TRP:HE3  | 1:167:A:ALA:HB3  | 6        | 0.66          |
| (1,71)   | 1:95:A:TRP:HB3  | 1:168:A:PRO:HB2  | 4        | 0.66          |
| (1,4296) | 1:173:B:ALA:H   | 1:172:B:LEU:HG   | 10       | 0.65          |
| (1,4285) | 1:171:B:LYS:H   | 1:169:B:MET:HA   | 9        | 0.65          |
| (1,4267) | 1:167:B:ALA:H   | 1:169:B:MET:H    | 8        | 0.65          |
| (1,3911) | 1:129:B:ASP:H   | 1:133:B:TYR:HD1  | 4        | 0.65          |
| (1,3911) | 1:129:B:ASP:H   | 1:133:B:TYR:HD2  | 4        | 0.65          |
| (1,3904) | 1:129:B:ASP:H   | 1:130:B:GLU:HG3  | 3        | 0.65          |
| (1,3437) | 1:157:B:LEU:HB2 | 1:163:B:LEU:HD11 | 8        | 0.65          |
| (1,3437) | 1:157:B:LEU:HB2 | 1:163:B:LEU:HD12 | 8        | 0.65          |
| (1,3437) | 1:157:B:LEU:HB2 | 1:163:B:LEU:HD13 | 8        | 0.65          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD21 | 6        | 0.65          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD22 | 6        | 0.65          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD23 | 6        | 0.65          |
| (1,3346) | 1:152:B:GLN:HB2 | 1:169:B:MET:HA   | 10       | 0.65          |
| (1,2996) | 1:126:B:GLU:HB2 | 1:135:B:SER:HB3  | 8        | 0.65          |
| (1,2986) | 1:126:B:GLU:HA  | 1:126:B:GLU:HG3  | 5        | 0.65          |
| (1,2970) | 1:123:B:LYS:HB3 | 1:137:B:CYS:HA   | 5        | 0.65          |
| (1,2643) | 1:109:B:LEU:HB3 | 1:121:B:THR:HB   | 3        | 0.65          |
| (1,2360) | 1:96:B:ARG:HA   | 1:96:B:ARG:HG3   | 4        | 0.65          |
| (1,2323) | 1:94:B:ARG:HB3  | 1:168:B:PRO:HA   | 5        | 0.65          |
| (1,2149) | 1:97:B:VAL:HG11 | 1:131:A:HIS:HB2  | 4        | 0.65          |
| (1,2149) | 1:97:B:VAL:HG12 | 1:131:A:HIS:HB2  | 4        | 0.65          |
| (1,2149) | 1:97:B:VAL:HG13 | 1:131:A:HIS:HB2  | 4        | 0.65          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2149) | 1:97:B:VAL:HG11 | 1:131:A:HIS:HB2  | 9        | 0.65          |
| (1,2149) | 1:97:B:VAL:HG12 | 1:131:A:HIS:HB2  | 9        | 0.65          |
| (1,2149) | 1:97:B:VAL:HG13 | 1:131:A:HIS:HB2  | 9        | 0.65          |
| (1,2017) | 1:97:B:VAL:HG11 | 1:131:A:HIS:HB2  | 4        | 0.65          |
| (1,2017) | 1:97:B:VAL:HG12 | 1:131:A:HIS:HB2  | 4        | 0.65          |
| (1,2017) | 1:97:B:VAL:HG13 | 1:131:A:HIS:HB2  | 4        | 0.65          |
| (1,2017) | 1:97:B:VAL:HG11 | 1:131:A:HIS:HB2  | 9        | 0.65          |
| (1,2017) | 1:97:B:VAL:HG12 | 1:131:A:HIS:HB2  | 9        | 0.65          |
| (1,2017) | 1:97:B:VAL:HG13 | 1:131:A:HIS:HB2  | 9        | 0.65          |
| (1,2004) | 1:171:A:LYS:H   | 1:169:A:MET:HA   | 5        | 0.65          |
| (1,1691) | 1:140:A:ARG:H   | 1:120:A:ILE:HB   | 2        | 0.65          |
| (1,1277) | 1:168:A:PRO:HA  | 1:169:A:MET:HG3  | 4        | 0.65          |
| (1,1140) | 1:156:A:SER:HB3 | 1:157:A:LEU:HD21 | 5        | 0.65          |
| (1,1140) | 1:156:A:SER:HB3 | 1:157:A:LEU:HD22 | 5        | 0.65          |
| (1,1140) | 1:156:A:SER:HB3 | 1:157:A:LEU:HD23 | 5        | 0.65          |
| (1,958)  | 1:145:A:PRO:HG3 | 1:146:A:PRO:HD2  | 1        | 0.65          |
| (1,958)  | 1:145:A:PRO:HG3 | 1:146:A:PRO:HD2  | 4        | 0.65          |
| (1,710)  | 1:126:A:GLU:HA  | 1:135:A:SER:HB2  | 3        | 0.65          |
| (1,514)  | 1:115:A:ASP:HB2 | 1:143:A:THR:HG21 | 2        | 0.65          |
| (1,514)  | 1:115:A:ASP:HB2 | 1:143:A:THR:HG22 | 2        | 0.65          |
| (1,514)  | 1:115:A:ASP:HB2 | 1:143:A:THR:HG23 | 2        | 0.65          |
| (1,4075) | 1:152:B:GLN:H   | 1:168:B:PRO:HD3  | 8        | 0.64          |
| (1,3763) | 1:114:B:LYS:H   | 1:115:B:ASP:HB2  | 4        | 0.64          |
| (1,3569) | 1:169:B:MET:HA  | 1:169:B:MET:HG2  | 6        | 0.64          |
| (1,3473) | 1:158:B:SER:HB2 | 1:162:B:THR:HB   | 2        | 0.64          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD21 | 4        | 0.64          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD22 | 4        | 0.64          |
| (1,3421) | 1:156:B:SER:HB3 | 1:157:B:LEU:HD23 | 4        | 0.64          |
| (1,3035) | 1:128:B:GLN:HB2 | 1:133:B:TYR:HE1  | 1        | 0.64          |
| (1,3035) | 1:128:B:GLN:HB2 | 1:133:B:TYR:HE2  | 1        | 0.64          |
| (1,2755) | 1:112:B:LYS:HE2 | 1:114:B:LYS:HB3  | 7        | 0.64          |
| (1,2436) | 1:97:B:VAL:HG21 | 1:144:B:LEU:HB2  | 2        | 0.64          |
| (1,2436) | 1:97:B:VAL:HG22 | 1:144:B:LEU:HB2  | 2        | 0.64          |
| (1,2436) | 1:97:B:VAL:HG23 | 1:144:B:LEU:HB2  | 2        | 0.64          |
| (1,2360) | 1:96:B:ARG:HA   | 1:96:B:ARG:HG3   | 2        | 0.64          |
| (1,2287) | 1:90:B:HIS:HA   | 1:91:B:THR:HG21  | 2        | 0.64          |
| (1,2287) | 1:90:B:HIS:HA   | 1:91:B:THR:HG22  | 2        | 0.64          |
| (1,2287) | 1:90:B:HIS:HA   | 1:91:B:THR:HG23  | 2        | 0.64          |
| (1,2284) | 1:89:B:ARG:HB2  | 1:90:B:HIS:HB2   | 10       | 0.64          |
| (1,2282) | 1:88:B:ILE:HG21 | 1:90:B:HIS:HA    | 9        | 0.64          |
| (1,2282) | 1:88:B:ILE:HG22 | 1:90:B:HIS:HA    | 9        | 0.64          |
| (1,2282) | 1:88:B:ILE:HG23 | 1:90:B:HIS:HA    | 9        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 8        | 0.64          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 4        | 0.64          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 4        | 0.64          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 4        | 0.64          |
| (1,1322) | 1:94:A:ARG:H     | 1:93:A:ASP:HB2   | 6        | 0.64          |
| (1,1288) | 1:169:A:MET:HA   | 1:169:A:MET:HG2  | 9        | 0.64          |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 1        | 0.64          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 8        | 0.64          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 3        | 0.64          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 8        | 0.64          |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 5        | 0.64          |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD3  | 8        | 0.64          |
| (1,4255) | 1:167:B:ALA:H    | 1:95:B:TRP:HB3   | 7        | 0.63          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 4        | 0.63          |
| (1,3603) | 1:94:B:ARG:H     | 1:93:B:ASP:HB2   | 1        | 0.63          |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 9        | 0.63          |
| (1,3013) | 1:126:B:GLU:HG3  | 1:134:B:ILE:HG22 | 7        | 0.63          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 2        | 0.63          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 2        | 0.63          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 2        | 0.63          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 4        | 0.63          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 10       | 0.63          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 3        | 0.63          |
| (1,2314) | 1:94:B:ARG:HA    | 1:169:B:MET:HB2  | 6        | 0.63          |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB1   | 4        | 0.63          |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB2   | 4        | 0.63          |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB3   | 4        | 0.63          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 3        | 0.63          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 1        | 0.63          |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG21 | 5        | 0.63          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG21  | 6        | 0.63          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG22  | 6        | 0.63          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG23  | 6        | 0.63          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 5        | 0.63          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 7        | 0.63          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG21 | 5        | 0.63          |
| (1,695)  | 1:123:A:LYS:HD2  | 1:137:A:CYS:HB2  | 1        | 0.63          |
| (1,406)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HE3  | 8        | 0.63          |
| (1,406)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HE3  | 8        | 0.63          |
| (1,406)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HE3  | 8        | 0.63          |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 10       | 0.63          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 10       | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 10       | 0.63          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 7        | 0.63          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 2        | 0.63          |
| (1,7)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HA    | 2        | 0.63          |
| (1,4048) | 1:149:B:ASP:H    | 1:170:B:PRO:HG3  | 4        | 0.62          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 7        | 0.62          |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 9        | 0.62          |
| (1,3569) | 1:169:B:MET:HA   | 1:169:B:MET:HG2  | 3        | 0.62          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD11 | 3        | 0.62          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD12 | 3        | 0.62          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD13 | 3        | 0.62          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 10       | 0.62          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 10       | 0.62          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 10       | 0.62          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 6        | 0.62          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 6        | 0.62          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 6        | 0.62          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 9        | 0.62          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 1        | 0.62          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 1        | 0.62          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 1        | 0.62          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 7        | 0.62          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 7        | 0.62          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 7        | 0.62          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 1        | 0.62          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 3        | 0.62          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 3        | 0.62          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 3        | 0.62          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 6        | 0.62          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 6        | 0.62          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 6        | 0.62          |
| (1,2513) | 1:99:B:LEU:HD11  | 1:120:B:ILE:HG12 | 6        | 0.62          |
| (1,2513) | 1:99:B:LEU:HD12  | 1:120:B:ILE:HG12 | 6        | 0.62          |
| (1,2513) | 1:99:B:LEU:HD13  | 1:120:B:ILE:HG12 | 6        | 0.62          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 9        | 0.62          |
| (1,2290) | 1:90:B:HIS:HB3   | 1:91:B:THR:HA    | 8        | 0.62          |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD3  | 10       | 0.62          |
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD3  | 10       | 0.62          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD3   | 2        | 0.62          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB3   | 8        | 0.62          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 1        | 0.62          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 1        | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 1        | 0.62          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 3        | 0.62          |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG3  | 9        | 0.62          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 7        | 0.62          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 7        | 0.62          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 7        | 0.62          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 7        | 0.62          |
| (1,1114) | 1:155:A:SER:HB2  | 1:163:A:LEU:HA   | 2        | 0.62          |
| (1,743)  | 1:127:A:ARG:HB3  | 1:127:A:ARG:HD2  | 5        | 0.62          |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 6        | 0.62          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE1  | 10       | 0.62          |
| (1,642)  | 1:120:A:ILE:HG13 | 1:142:A:TYR:HE2  | 10       | 0.62          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 7        | 0.62          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 7        | 0.62          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 7        | 0.62          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 9        | 0.62          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 9        | 0.62          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 9        | 0.62          |
| (1,31)   | 1:94:A:ARG:HA    | 1:168:A:PRO:HD2  | 2        | 0.62          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 2        | 0.61          |
| (1,4080) | 1:152:B:GLN:HE21 | 1:152:B:GLN:HB3  | 10       | 0.61          |
| (1,4024) | 1:148:B:VAL:H    | 1:146:B:PRO:HB3  | 5        | 0.61          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG23 | 9        | 0.61          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 2        | 0.61          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 2        | 0.61          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 2        | 0.61          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 5        | 0.61          |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 10       | 0.61          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 6        | 0.61          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 8        | 0.61          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 8        | 0.61          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 8        | 0.61          |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 7        | 0.61          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 10       | 0.61          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 10       | 0.61          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 10       | 0.61          |
| (1,3118) | 1:140:B:ARG:HA   | 1:140:B:ARG:HD3  | 3        | 0.61          |
| (1,3116) | 1:139:B:THR:HG21 | 1:141:B:LYS:HE2  | 7        | 0.61          |
| (1,3116) | 1:139:B:THR:HG22 | 1:141:B:LYS:HE2  | 7        | 0.61          |
| (1,3116) | 1:139:B:THR:HG23 | 1:141:B:LYS:HE2  | 7        | 0.61          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 2        | 0.61          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 5        | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 5        | 0.61          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 5        | 0.61          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG21 | 5        | 0.61          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG22 | 5        | 0.61          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG23 | 5        | 0.61          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG21 | 8        | 0.61          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG22 | 8        | 0.61          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG23 | 8        | 0.61          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 4        | 0.61          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 4        | 0.61          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 4        | 0.61          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 7        | 0.61          |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 5        | 0.61          |
| (1,2013) | 1:172:A:LEU:H    | 1:172:A:LEU:HB2  | 10       | 0.61          |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HD13 | 10       | 0.61          |
| (1,1413) | 1:108:A:GLU:H    | 1:106:A:PRO:HB3  | 7        | 0.61          |
| (1,1288) | 1:169:A:MET:HA   | 1:169:A:MET:HG2  | 1        | 0.61          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 8        | 0.61          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 8        | 0.61          |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 8        | 0.61          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 3        | 0.61          |
| (1,968)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA3  | 3        | 0.61          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 5        | 0.61          |
| (1,958)  | 1:145:A:PRO:HG3  | 1:146:A:PRO:HD2  | 7        | 0.61          |
| (1,958)  | 1:145:A:PRO:HG3  | 1:146:A:PRO:HD2  | 8        | 0.61          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 6        | 0.61          |
| (1,474)  | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB3  | 4        | 0.61          |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD2  | 10       | 0.61          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 1        | 0.61          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 1        | 0.61          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 1        | 0.61          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 1        | 0.61          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 10       | 0.61          |
| (1,72)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB3  | 10       | 0.61          |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 10       | 0.6           |
| (1,3972) | 1:140:B:ARG:H    | 1:120:B:ILE:HB   | 2        | 0.6           |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG23 | 4        | 0.6           |
| (1,3904) | 1:129:B:ASP:H    | 1:130:B:GLU:HG3  | 1        | 0.6           |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 4        | 0.6           |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 2        | 0.6           |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 2        | 0.6           |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 2        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 2        | 0.6           |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 5        | 0.6           |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 5        | 0.6           |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 5        | 0.6           |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 4        | 0.6           |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 4        | 0.6           |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 4        | 0.6           |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 3        | 0.6           |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 3        | 0.6           |
| (1,2996) | 1:126:B:GLU:HB2  | 1:135:B:SER:HB3  | 4        | 0.6           |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 8        | 0.6           |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 8        | 0.6           |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 8        | 0.6           |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1  | 9        | 0.6           |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2  | 9        | 0.6           |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 3        | 0.6           |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 3        | 0.6           |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 3        | 0.6           |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 2        | 0.6           |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 3        | 0.6           |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 6        | 0.6           |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 6        | 0.6           |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 6        | 0.6           |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 8        | 0.6           |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 8        | 0.6           |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 8        | 0.6           |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 6        | 0.6           |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 6        | 0.6           |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 6        | 0.6           |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 8        | 0.6           |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 8        | 0.6           |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 8        | 0.6           |
| (1,1916) | 1:162:A:THR:H    | 1:102:A:ASN:HB3  | 4        | 0.6           |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 6        | 0.6           |
| (1,1656) | 1:134:A:ILE:H    | 1:127:A:ARG:HG3  | 1        | 0.6           |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 1        | 0.6           |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 10       | 0.6           |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 10       | 0.6           |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 10       | 0.6           |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 9        | 0.6           |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 4        | 0.6           |
| (1,845)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HD2  | 9        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,723)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB2  | 4        | 0.6           |
| (1,723)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB2  | 8        | 0.6           |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 3        | 0.6           |
| (1,682)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HE3  | 7        | 0.6           |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 3        | 0.6           |
| (1,4267) | 1:167:B:ALA:H    | 1:169:B:MET:H    | 7        | 0.59          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 10       | 0.59          |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 7        | 0.59          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 1        | 0.59          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 1        | 0.59          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 1        | 0.59          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 4        | 0.59          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 5        | 0.59          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 5        | 0.59          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 8        | 0.59          |
| (1,2907) | 1:120:B:ILE:HA   | 1:120:B:ILE:HG13 | 4        | 0.59          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 9        | 0.59          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 2        | 0.59          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 2        | 0.59          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 2        | 0.59          |
| (1,2625) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HD2  | 4        | 0.59          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD21 | 9        | 0.59          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD22 | 9        | 0.59          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD23 | 9        | 0.59          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 8        | 0.59          |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 8        | 0.59          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 8        | 0.59          |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 8        | 0.59          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 8        | 0.59          |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 8        | 0.59          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 1        | 0.59          |
| (1,2346) | 1:95:B:TRP:HB3   | 1:95:B:TRP:HE3   | 1        | 0.59          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 10       | 0.59          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 10       | 0.59          |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG23 | 3        | 0.59          |
| (1,1623) | 1:129:A:ASP:H    | 1:130:A:GLU:HG3  | 9        | 0.59          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 3        | 0.59          |
| (1,1277) | 1:168:A:PRO:HA   | 1:169:A:MET:HG3  | 3        | 0.59          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD21 | 10       | 0.59          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD22 | 10       | 0.59          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD23 | 10       | 0.59          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 2        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG22 | 1        | 0.59          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 2        | 0.59          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 9        | 0.59          |
| (1,626)  | 1:120:A:ILE:HA   | 1:120:A:ILE:HG13 | 3        | 0.59          |
| (1,257)  | 1:99:A:LEU:HD11  | 1:112:A:LYS:HG3  | 6        | 0.59          |
| (1,257)  | 1:99:A:LEU:HD12  | 1:112:A:LYS:HG3  | 6        | 0.59          |
| (1,257)  | 1:99:A:LEU:HD13  | 1:112:A:LYS:HG3  | 6        | 0.59          |
| (1,232)  | 1:99:A:LEU:HD11  | 1:120:A:ILE:HG12 | 9        | 0.59          |
| (1,232)  | 1:99:A:LEU:HD12  | 1:120:A:ILE:HG12 | 9        | 0.59          |
| (1,232)  | 1:99:A:LEU:HD13  | 1:120:A:ILE:HG12 | 9        | 0.59          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 3        | 0.59          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 3        | 0.59          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 3        | 0.59          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB1   | 9        | 0.59          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB2   | 9        | 0.59          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB3   | 9        | 0.59          |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD3   | 10       | 0.58          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG23 | 3        | 0.58          |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 1        | 0.58          |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 6        | 0.58          |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 4        | 0.58          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 10       | 0.58          |
| (1,3249) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA3  | 9        | 0.58          |
| (1,3248) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA2  | 6        | 0.58          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 5        | 0.58          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 5        | 0.58          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 5        | 0.58          |
| (1,3126) | 1:141:B:LYS:HA   | 1:141:B:LYS:HD3  | 5        | 0.58          |
| (1,3126) | 1:141:B:LYS:HA   | 1:141:B:LYS:HD2  | 7        | 0.58          |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 3        | 0.58          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 6        | 0.58          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 2        | 0.58          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 3        | 0.58          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 7        | 0.58          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 7        | 0.58          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 7        | 0.58          |
| (1,2930) | 1:120:B:ILE:HG21 | 1:140:B:ARG:HA   | 6        | 0.58          |
| (1,2930) | 1:120:B:ILE:HG22 | 1:140:B:ARG:HA   | 6        | 0.58          |
| (1,2930) | 1:120:B:ILE:HG23 | 1:140:B:ARG:HA   | 6        | 0.58          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE2  | 5        | 0.58          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 8        | 0.58          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 8        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 8        | 0.58          |
| (1,2608) | 1:106:B:PRO:HG3  | 1:157:B:LEU:HD11 | 10       | 0.58          |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 9        | 0.58          |
| (1,2283) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HB3   | 8        | 0.58          |
| (1,2283) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HB3   | 8        | 0.58          |
| (1,2283) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HB3   | 8        | 0.58          |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 7        | 0.58          |
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 1        | 0.58          |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE1  | 8        | 0.58          |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE2  | 8        | 0.58          |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 9        | 0.58          |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 9        | 0.58          |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 9        | 0.58          |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 1        | 0.58          |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 1        | 0.58          |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 1        | 0.58          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 2        | 0.58          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 2        | 0.58          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 2        | 0.58          |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 8        | 0.58          |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 8        | 0.58          |
| (1,16)   | 1:93:A:ASP:HA    | 1:94:A:ARG:HD2   | 1        | 0.58          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB3   | 1        | 0.57          |
| (1,4025) | 1:148:B:VAL:H    | 1:146:B:PRO:HG2  | 5        | 0.57          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG22 | 1        | 0.57          |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 4        | 0.57          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 1        | 0.57          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 1        | 0.57          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 1        | 0.57          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 2        | 0.57          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 2        | 0.57          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 2        | 0.57          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 6        | 0.57          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 6        | 0.57          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 6        | 0.57          |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 5        | 0.57          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 8        | 0.57          |
| (1,3005) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB3  | 8        | 0.57          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 3        | 0.57          |
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 2        | 0.57          |
| (1,2907) | 1:120:B:ILE:HA   | 1:120:B:ILE:HG13 | 8        | 0.57          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 1        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 1        | 0.57          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 1        | 0.57          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 8        | 0.57          |
| (1,2346) | 1:95:B:TRP:HB3   | 1:95:B:TRP:HE3   | 7        | 0.57          |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 10       | 0.57          |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 8        | 0.57          |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 10       | 0.57          |
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 8        | 0.57          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 3        | 0.57          |
| (1,1691) | 1:140:A:ARG:H    | 1:120:A:ILE:HB   | 7        | 0.57          |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG3  | 7        | 0.57          |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 7        | 0.57          |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 5        | 0.57          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 9        | 0.57          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 9        | 0.57          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 9        | 0.57          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 5        | 0.57          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 4        | 0.57          |
| (1,805)  | 1:134:A:ILE:HD11 | 1:135:A:SER:HB2  | 1        | 0.57          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 2        | 0.57          |
| (1,733)  | 1:126:A:GLU:HG3  | 1:135:A:SER:HB3  | 3        | 0.57          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 5        | 0.57          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 5        | 0.57          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 5        | 0.57          |
| (1,65)   | 1:95:A:TRP:HB3   | 1:95:A:TRP:HE3   | 7        | 0.57          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB1   | 7        | 0.57          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB2   | 7        | 0.57          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB3   | 7        | 0.57          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 10       | 0.56          |
| (1,4095) | 1:152:B:GLN:HE22 | 1:170:B:PRO:HD3  | 3        | 0.56          |
| (1,4080) | 1:152:B:GLN:HE21 | 1:152:B:GLN:HB3  | 9        | 0.56          |
| (1,4024) | 1:148:B:VAL:H    | 1:146:B:PRO:HB3  | 6        | 0.56          |
| (1,3972) | 1:140:B:ARG:H    | 1:120:B:ILE:HB   | 3        | 0.56          |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG3  | 1        | 0.56          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD1  | 2        | 0.56          |
| (1,3911) | 1:129:B:ASP:H    | 1:133:B:TYR:HD2  | 2        | 0.56          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 1        | 0.56          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 7        | 0.56          |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 6        | 0.56          |
| (1,3293) | 1:148:B:VAL:HG11 | 1:169:B:MET:HB2  | 4        | 0.56          |
| (1,3293) | 1:148:B:VAL:HG12 | 1:169:B:MET:HB2  | 4        | 0.56          |
| (1,3293) | 1:148:B:VAL:HG13 | 1:169:B:MET:HB2  | 4        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 3        | 0.56          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 9        | 0.56          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 7        | 0.56          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 5        | 0.56          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 5        | 0.56          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 5        | 0.56          |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD2  | 10       | 0.56          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 8        | 0.56          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 3        | 0.56          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 10       | 0.56          |
| (1,2169) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 9        | 0.56          |
| (1,2037) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 9        | 0.56          |
| (1,1916) | 1:162:A:THR:H    | 1:102:A:ASN:HB3  | 2        | 0.56          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 2        | 0.56          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 4        | 0.56          |
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 7        | 0.56          |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 8        | 0.56          |
| (1,1114) | 1:155:A:SER:HB2  | 1:163:A:LEU:HA   | 1        | 0.56          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 3        | 0.56          |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 2        | 0.56          |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 10       | 0.56          |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 9        | 0.56          |
| (1,626)  | 1:120:A:ILE:HA   | 1:120:A:ILE:HG13 | 1        | 0.56          |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 6        | 0.56          |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 6        | 0.56          |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 6        | 0.56          |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD3  | 1        | 0.56          |
| (1,255)  | 1:99:A:LEU:HD21  | 1:109:A:LEU:HG   | 4        | 0.56          |
| (1,255)  | 1:99:A:LEU:HD22  | 1:109:A:LEU:HG   | 4        | 0.56          |
| (1,255)  | 1:99:A:LEU:HD23  | 1:109:A:LEU:HG   | 4        | 0.56          |
| (1,104)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HA   | 3        | 0.56          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 2        | 0.56          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 2        | 0.56          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 2        | 0.56          |
| (1,65)   | 1:95:A:TRP:HB3   | 1:95:A:TRP:HE3   | 4        | 0.56          |
| (1,33)   | 1:94:A:ARG:HA    | 1:169:A:MET:HB2  | 2        | 0.56          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 8        | 0.56          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 6        | 0.55          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 5        | 0.55          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 5        | 0.55          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 5        | 0.55          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 5        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD3  | 6        | 0.55          |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 5        | 0.55          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 10       | 0.55          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 3        | 0.55          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 3        | 0.55          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 3        | 0.55          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG23 | 8        | 0.55          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG22 | 10       | 0.55          |
| (1,2907) | 1:120:B:ILE:HA   | 1:120:B:ILE:HG13 | 7        | 0.55          |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE3  | 5        | 0.55          |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE3  | 5        | 0.55          |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE3  | 5        | 0.55          |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE3  | 6        | 0.55          |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE3  | 6        | 0.55          |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE3  | 6        | 0.55          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 3        | 0.55          |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 3        | 0.55          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 3        | 0.55          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 6        | 0.55          |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 6        | 0.55          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 6        | 0.55          |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 3        | 0.55          |
| (1,2313) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD3  | 2        | 0.55          |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 7        | 0.55          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 2        | 0.55          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 9        | 0.55          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 10       | 0.55          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 6        | 0.55          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 6        | 0.55          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 6        | 0.55          |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 8        | 0.55          |
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 3        | 0.55          |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 9        | 0.55          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 9        | 0.55          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 6        | 0.55          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 6        | 0.55          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 6        | 0.55          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 1        | 0.55          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 7        | 0.55          |
| (1,770)  | 1:129:A:ASP:HB3  | 1:130:A:GLU:HA   | 8        | 0.55          |
| (1,723)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB2  | 1        | 0.55          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 1        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,626)  | 1:120:A:ILE:HA   | 1:120:A:ILE:HG13 | 8        | 0.55          |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 5        | 0.55          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 5        | 0.55          |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 5        | 0.55          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 8        | 0.55          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 8        | 0.55          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 8        | 0.55          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB1  | 8        | 0.55          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB2  | 8        | 0.55          |
| (1,77)   | 1:95:A:TRP:HE3   | 1:167:A:ALA:HB3  | 8        | 0.55          |
| (1,4280) | 1:169:B:MET:H    | 1:169:B:MET:HB3  | 2        | 0.54          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 7        | 0.54          |
| (1,4084) | 1:152:B:GLN:HE21 | 1:168:B:PRO:HD2  | 3        | 0.54          |
| (1,4036) | 1:148:B:VAL:H    | 1:170:B:PRO:HB2  | 9        | 0.54          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 8        | 0.54          |
| (1,3603) | 1:94:B:ARG:H     | 1:93:B:ASP:HB2   | 8        | 0.54          |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD3  | 10       | 0.54          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 6        | 0.54          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 6        | 0.54          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 6        | 0.54          |
| (1,3137) | 1:141:B:LYS:HG2  | 1:142:B:TYR:HB3  | 10       | 0.54          |
| (1,3126) | 1:141:B:LYS:HA   | 1:141:B:LYS:HD2  | 6        | 0.54          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 9        | 0.54          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 9        | 0.54          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 10       | 0.54          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 1        | 0.54          |
| (1,2715) | 1:111:B:VAL:HG11 | 1:120:B:ILE:HG12 | 6        | 0.54          |
| (1,2715) | 1:111:B:VAL:HG12 | 1:120:B:ILE:HG12 | 6        | 0.54          |
| (1,2715) | 1:111:B:VAL:HG13 | 1:120:B:ILE:HG12 | 6        | 0.54          |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 9        | 0.54          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 9        | 0.54          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 9        | 0.54          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD21 | 3        | 0.54          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD22 | 3        | 0.54          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD23 | 3        | 0.54          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 5        | 0.54          |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 5        | 0.54          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 5        | 0.54          |
| (1,2299) | 1:93:B:ASP:HB2   | 1:94:B:ARG:HA    | 3        | 0.54          |
| (1,2193) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 5        | 0.54          |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 1        | 0.54          |
| (1,2061) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD2  | 5        | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 1        | 0.54          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 7        | 0.54          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 9        | 0.54          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 9        | 0.54          |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 7        | 0.54          |
| (1,1756) | 1:148:A:VAL:H    | 1:170:A:PRO:HG3  | 7        | 0.54          |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD13 | 7        | 0.54          |
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 5        | 0.54          |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 7        | 0.54          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 3        | 0.54          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 3        | 0.54          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 3        | 0.54          |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 10       | 0.54          |
| (1,626)  | 1:120:A:ILE:HA   | 1:120:A:ILE:HG13 | 5        | 0.54          |
| (1,626)  | 1:120:A:ILE:HA   | 1:120:A:ILE:HG13 | 10       | 0.54          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD11 | 1        | 0.54          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD12 | 1        | 0.54          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD13 | 1        | 0.54          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 8        | 0.54          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 8        | 0.54          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 8        | 0.54          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 6        | 0.54          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 6        | 0.54          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 6        | 0.54          |
| (1,65)   | 1:95:A:TRP:HB3   | 1:95:A:TRP:HE3   | 10       | 0.54          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 3        | 0.53          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 5        | 0.53          |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 9        | 0.53          |
| (1,4025) | 1:148:B:VAL:H    | 1:146:B:PRO:HG2  | 6        | 0.53          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 6        | 0.53          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 4        | 0.53          |
| (1,3491) | 1:160:B:GLU:HB2  | 1:162:B:THR:HB   | 10       | 0.53          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 7        | 0.53          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 7        | 0.53          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 7        | 0.53          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 5        | 0.53          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD21 | 7        | 0.53          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD22 | 7        | 0.53          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD23 | 7        | 0.53          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD11 | 10       | 0.53          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD12 | 10       | 0.53          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD13 | 10       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 1        | 0.53          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 4        | 0.53          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 7        | 0.53          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 7        | 0.53          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 7        | 0.53          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 5        | 0.53          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 5        | 0.53          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 5        | 0.53          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 9        | 0.53          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 10       | 0.53          |
| (1,2980) | 1:125:B:GLU:HA   | 1:125:B:GLU:HG2  | 7        | 0.53          |
| (1,2907) | 1:120:B:ILE:HA   | 1:120:B:ILE:HG13 | 1        | 0.53          |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE3  | 2        | 0.53          |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE3  | 2        | 0.53          |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE3  | 2        | 0.53          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 6        | 0.53          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 6        | 0.53          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 6        | 0.53          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 10       | 0.53          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 10       | 0.53          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 10       | 0.53          |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 2        | 0.53          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 10       | 0.53          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD21 | 5        | 0.53          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD22 | 5        | 0.53          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD23 | 5        | 0.53          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 7        | 0.53          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 9        | 0.53          |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 9        | 0.53          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 9        | 0.53          |
| (1,2000) | 1:169:A:MET:H    | 1:169:A:MET:HG3  | 2        | 0.53          |
| (1,1691) | 1:140:A:ARG:H    | 1:120:A:ILE:HB   | 4        | 0.53          |
| (1,1514) | 1:118:A:VAL:H    | 1:119:A:GLU:HG3  | 1        | 0.53          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 7        | 0.53          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 7        | 0.53          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 7        | 0.53          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD21 | 8        | 0.53          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD22 | 8        | 0.53          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD23 | 8        | 0.53          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 5        | 0.53          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 5        | 0.53          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 5        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 10       | 0.53          |
| (1,721)  | 1:126:A:GLU:HG2  | 1:134:A:ILE:HG22 | 9        | 0.53          |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 3        | 0.53          |
| (1,688)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB3  | 8        | 0.53          |
| (1,509)  | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 10       | 0.53          |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 1        | 0.53          |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 1        | 0.53          |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 1        | 0.53          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 6        | 0.53          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 6        | 0.53          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 6        | 0.53          |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 6        | 0.53          |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 6        | 0.53          |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 6        | 0.53          |
| (1,255)  | 1:99:A:LEU:HD21  | 1:109:A:LEU:HG   | 6        | 0.53          |
| (1,255)  | 1:99:A:LEU:HD22  | 1:109:A:LEU:HG   | 6        | 0.53          |
| (1,255)  | 1:99:A:LEU:HD23  | 1:109:A:LEU:HG   | 6        | 0.53          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 4        | 0.53          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 2        | 0.52          |
| (1,4093) | 1:152:B:GLN:HE22 | 1:168:B:PRO:HD3  | 2        | 0.52          |
| (1,3895) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB2  | 3        | 0.52          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 5        | 0.52          |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD13 | 7        | 0.52          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 2        | 0.52          |
| (1,3612) | 1:95:B:TRP:H     | 1:95:B:TRP:HB2   | 9        | 0.52          |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD3  | 5        | 0.52          |
| (1,3491) | 1:160:B:GLU:HB2  | 1:162:B:THR:HB   | 8        | 0.52          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 8        | 0.52          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 2        | 0.52          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 2        | 0.52          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 2        | 0.52          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD11 | 5        | 0.52          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD12 | 5        | 0.52          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD13 | 5        | 0.52          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 4        | 0.52          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 4        | 0.52          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 4        | 0.52          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG21 | 3        | 0.52          |
| (1,2975) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HA   | 7        | 0.52          |
| (1,2974) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB3  | 6        | 0.52          |
| (1,2971) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HB2  | 10       | 0.52          |
| (1,2907) | 1:120:B:ILE:HA   | 1:120:B:ILE:HG13 | 9        | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 5        | 0.52          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD21 | 2        | 0.52          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD22 | 2        | 0.52          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD23 | 2        | 0.52          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 4        | 0.52          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD11 | 1        | 0.52          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD12 | 1        | 0.52          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD13 | 1        | 0.52          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 6        | 0.52          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 9        | 0.52          |
| (1,2346) | 1:95:B:TRP:HB3   | 1:95:B:TRP:HE3   | 8        | 0.52          |
| (1,2200) | 1:134:B:ILE:HG21 | 1:140:A:ARG:HD3  | 3        | 0.52          |
| (1,2200) | 1:134:B:ILE:HG22 | 1:140:A:ARG:HD3  | 3        | 0.52          |
| (1,2200) | 1:134:B:ILE:HG23 | 1:140:A:ARG:HD3  | 3        | 0.52          |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 10       | 0.52          |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 10       | 0.52          |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 10       | 0.52          |
| (1,2068) | 1:134:B:ILE:HG21 | 1:140:A:ARG:HD3  | 3        | 0.52          |
| (1,2068) | 1:134:B:ILE:HG22 | 1:140:A:ARG:HD3  | 3        | 0.52          |
| (1,2068) | 1:134:B:ILE:HG23 | 1:140:A:ARG:HD3  | 3        | 0.52          |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 10       | 0.52          |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 10       | 0.52          |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 10       | 0.52          |
| (1,1642) | 1:132:A:GLY:H    | 1:129:A:ASP:HB2  | 2        | 0.52          |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 3        | 0.52          |
| (1,1210) | 1:160:A:GLU:HB2  | 1:162:A:THR:HB   | 4        | 0.52          |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 6        | 0.52          |
| (1,694)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HA   | 4        | 0.52          |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 4        | 0.52          |
| (1,280)  | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA3  | 1        | 0.52          |
| (1,255)  | 1:99:A:LEU:HD21  | 1:109:A:LEU:HG   | 7        | 0.52          |
| (1,255)  | 1:99:A:LEU:HD22  | 1:109:A:LEU:HG   | 7        | 0.52          |
| (1,255)  | 1:99:A:LEU:HD23  | 1:109:A:LEU:HG   | 7        | 0.52          |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 10       | 0.52          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 6        | 0.52          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 10       | 0.52          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 7        | 0.52          |
| (1,72)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB3  | 7        | 0.52          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 2        | 0.52          |
| (1,4262) | 1:167:B:ALA:H    | 1:166:B:GLU:HB2  | 6        | 0.51          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 7        | 0.51          |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 4        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 7        | 0.51          |
| (1,3889) | 1:128:B:GLN:HE22 | 1:128:B:GLN:HB2  | 10       | 0.51          |
| (1,3848) | 1:123:B:LYS:H    | 1:109:B:LEU:HG   | 6        | 0.51          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 6        | 0.51          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 6        | 0.51          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 6        | 0.51          |
| (1,3613) | 1:95:B:TRP:H     | 1:95:B:TRP:HE3   | 7        | 0.51          |
| (1,3604) | 1:94:B:ARG:H     | 1:93:B:ASP:HB3   | 7        | 0.51          |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 4        | 0.51          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 1        | 0.51          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 1        | 0.51          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 1        | 0.51          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 10       | 0.51          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 10       | 0.51          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 10       | 0.51          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 8        | 0.51          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 8        | 0.51          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 8        | 0.51          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 4        | 0.51          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 4        | 0.51          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 4        | 0.51          |
| (1,2993) | 1:126:B:GLU:HB2  | 1:133:B:TYR:HB2  | 4        | 0.51          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE1  | 3        | 0.51          |
| (1,2923) | 1:120:B:ILE:HG13 | 1:142:B:TYR:HE2  | 3        | 0.51          |
| (1,2907) | 1:120:B:ILE:HA   | 1:120:B:ILE:HG13 | 10       | 0.51          |
| (1,2759) | 1:112:B:LYS:HE2  | 1:121:B:THR:HB   | 6        | 0.51          |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 3        | 0.51          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 1        | 0.51          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 1        | 0.51          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 8        | 0.51          |
| (1,2282) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HA    | 10       | 0.51          |
| (1,2282) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HA    | 10       | 0.51          |
| (1,2282) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HA    | 10       | 0.51          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 8        | 0.51          |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 5        | 0.51          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 8        | 0.51          |
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 5        | 0.51          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD3   | 5        | 0.51          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 6        | 0.51          |
| (1,1799) | 1:152:A:GLN:HE21 | 1:152:A:GLN:HB3  | 7        | 0.51          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 10       | 0.51          |
| (1,1193) | 1:158:A:SER:HB3  | 1:160:A:GLU:HB3  | 2        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 10       | 0.51          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 7        | 0.51          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD21 | 9        | 0.51          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD22 | 9        | 0.51          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD23 | 9        | 0.51          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 8        | 0.51          |
| (1,722)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HA   | 6        | 0.51          |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 8        | 0.51          |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 1        | 0.51          |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 6        | 0.51          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 4        | 0.51          |
| (1,449)  | 1:112:A:LYS:HA   | 1:112:A:LYS:HE3  | 9        | 0.51          |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 7        | 0.51          |
| (1,359)  | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 4        | 0.51          |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD3  | 9        | 0.51          |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 3        | 0.51          |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 7        | 0.51          |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 8        | 0.51          |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 6        | 0.51          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 4        | 0.51          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 2        | 0.51          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 2        | 0.51          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 2        | 0.51          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 1        | 0.51          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 1        | 0.51          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 1        | 0.51          |
| (1,18)   | 1:93:A:ASP:HB2   | 1:94:A:ARG:HA    | 6        | 0.51          |
| (1,4269) | 1:169:B:MET:H    | 1:94:B:ARG:HA    | 7        | 0.5           |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 10       | 0.5           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB1  | 7        | 0.5           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB2  | 7        | 0.5           |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB3  | 7        | 0.5           |
| (1,4095) | 1:152:B:GLN:HE22 | 1:170:B:PRO:HD3  | 1        | 0.5           |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 10       | 0.5           |
| (1,4024) | 1:148:B:VAL:H    | 1:146:B:PRO:HB3  | 8        | 0.5           |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG21 | 5        | 0.5           |
| (1,3763) | 1:114:B:LYS:H    | 1:115:B:ASP:HB2  | 7        | 0.5           |
| (1,3704) | 1:108:B:GLU:H    | 1:123:B:LYS:HG2  | 2        | 0.5           |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 3        | 0.5           |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD11 | 6        | 0.5           |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD12 | 6        | 0.5           |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD13 | 6        | 0.5           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3420) | 1:156:B:SER:HB3 | 1:157:B:LEU:HB3  | 8        | 0.5           |
| (1,3400) | 1:155:B:SER:HB2 | 1:165:B:VAL:HA   | 7        | 0.5           |
| (1,3378) | 1:154:B:SER:HB3 | 1:155:B:SER:HA   | 6        | 0.5           |
| (1,3378) | 1:154:B:SER:HB3 | 1:155:B:SER:HA   | 10       | 0.5           |
| (1,3274) | 1:148:B:VAL:HA  | 1:170:B:PRO:HG2  | 3        | 0.5           |
| (1,3108) | 1:139:B:THR:HA  | 1:140:B:ARG:HG2  | 6        | 0.5           |
| (1,3107) | 1:139:B:THR:HA  | 1:140:B:ARG:HB2  | 1        | 0.5           |
| (1,3107) | 1:139:B:THR:HA  | 1:140:B:ARG:HB2  | 7        | 0.5           |
| (1,2993) | 1:126:B:GLU:HB2 | 1:133:B:TYR:HB2  | 8        | 0.5           |
| (1,2980) | 1:125:B:GLU:HA  | 1:125:B:GLU:HG2  | 5        | 0.5           |
| (1,2699) | 1:111:B:VAL:HA  | 1:120:B:ILE:HG12 | 6        | 0.5           |
| (1,2643) | 1:109:B:LEU:HB3 | 1:121:B:THR:HB   | 7        | 0.5           |
| (1,2616) | 1:107:B:ASP:HA  | 1:157:B:LEU:HD21 | 1        | 0.5           |
| (1,2616) | 1:107:B:ASP:HA  | 1:157:B:LEU:HD22 | 1        | 0.5           |
| (1,2616) | 1:107:B:ASP:HA  | 1:157:B:LEU:HD23 | 1        | 0.5           |
| (1,2616) | 1:107:B:ASP:HA  | 1:157:B:LEU:HD21 | 4        | 0.5           |
| (1,2616) | 1:107:B:ASP:HA  | 1:157:B:LEU:HD22 | 4        | 0.5           |
| (1,2616) | 1:107:B:ASP:HA  | 1:157:B:LEU:HD23 | 4        | 0.5           |
| (1,2563) | 1:105:B:ALA:HA  | 1:106:B:PRO:HB2  | 8        | 0.5           |
| (1,2473) | 1:98:B:SER:HB3  | 1:99:B:LEU:HD21  | 3        | 0.5           |
| (1,2473) | 1:98:B:SER:HB3  | 1:99:B:LEU:HD22  | 3        | 0.5           |
| (1,2473) | 1:98:B:SER:HB3  | 1:99:B:LEU:HD23  | 3        | 0.5           |
| (1,2349) | 1:95:B:TRP:HB3  | 1:148:B:VAL:HG21 | 4        | 0.5           |
| (1,2349) | 1:95:B:TRP:HB3  | 1:148:B:VAL:HG22 | 4        | 0.5           |
| (1,2349) | 1:95:B:TRP:HB3  | 1:148:B:VAL:HG23 | 4        | 0.5           |
| (1,2312) | 1:94:B:ARG:HA   | 1:168:B:PRO:HD2  | 1        | 0.5           |
| (1,2281) | 1:143:A:THR:H   | 1:132:B:GLY:HA2  | 3        | 0.5           |
| (1,2148) | 1:143:A:THR:H   | 1:132:B:GLY:HA2  | 3        | 0.5           |
| (1,2007) | 1:171:A:LYS:H   | 1:170:A:PRO:HD3  | 5        | 0.5           |
| (1,2000) | 1:169:A:MET:H   | 1:169:A:MET:HG3  | 9        | 0.5           |
| (1,1978) | 1:167:A:ALA:H   | 1:96:A:ARG:HD3   | 6        | 0.5           |
| (1,1654) | 1:134:A:ILE:H   | 1:127:A:ARG:HB2  | 3        | 0.5           |
| (1,1567) | 1:123:A:LYS:H   | 1:109:A:LEU:HG   | 2        | 0.5           |
| (1,1331) | 1:95:A:TRP:H    | 1:95:A:TRP:HB2   | 8        | 0.5           |
| (1,1322) | 1:94:A:ARG:H    | 1:93:A:ASP:HB2   | 4        | 0.5           |
| (1,1193) | 1:158:A:SER:HB3 | 1:160:A:GLU:HB3  | 4        | 0.5           |
| (1,1189) | 1:158:A:SER:HA  | 1:160:A:GLU:HB3  | 8        | 0.5           |
| (1,1100) | 1:154:A:SER:HB2 | 1:165:A:VAL:HG21 | 1        | 0.5           |
| (1,1100) | 1:154:A:SER:HB2 | 1:165:A:VAL:HG22 | 1        | 0.5           |
| (1,1100) | 1:154:A:SER:HB2 | 1:165:A:VAL:HG23 | 1        | 0.5           |
| (1,959)  | 1:145:A:PRO:HG3 | 1:148:A:VAL:HG11 | 2        | 0.5           |
| (1,959)  | 1:145:A:PRO:HG3 | 1:148:A:VAL:HG12 | 2        | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 2        | 0.5           |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 3        | 0.5           |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 6        | 0.5           |
| (1,712)  | 1:126:A:GLU:HB3  | 1:133:A:TYR:HB2  | 3        | 0.5           |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 7        | 0.5           |
| (1,695)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HB2  | 3        | 0.5           |
| (1,509)  | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 2        | 0.5           |
| (1,449)  | 1:112:A:LYS:HA   | 1:112:A:LYS:HE2  | 7        | 0.5           |
| (1,356)  | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 1        | 0.5           |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 2        | 0.5           |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 5        | 0.5           |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 9        | 0.5           |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 2        | 0.5           |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 2        | 0.5           |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 2        | 0.5           |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 7        | 0.5           |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 7        | 0.5           |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 7        | 0.5           |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 4        | 0.5           |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 4        | 0.5           |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 4        | 0.5           |
| (1,18)   | 1:93:A:ASP:HB2   | 1:94:A:ARG:HA    | 4        | 0.5           |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD2   | 9        | 0.49          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 8        | 0.49          |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 2        | 0.49          |
| (1,3460) | 1:157:B:LEU:HD21 | 1:163:B:LEU:HB3  | 7        | 0.49          |
| (1,3460) | 1:157:B:LEU:HD22 | 1:163:B:LEU:HB3  | 7        | 0.49          |
| (1,3460) | 1:157:B:LEU:HD23 | 1:163:B:LEU:HB3  | 7        | 0.49          |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 1        | 0.49          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 2        | 0.49          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 2        | 0.49          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 2        | 0.49          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 2        | 0.49          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG11 | 9        | 0.49          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG12 | 9        | 0.49          |
| (1,3240) | 1:145:B:PRO:HG3  | 1:148:B:VAL:HG13 | 9        | 0.49          |
| (1,3116) | 1:139:B:THR:HG21 | 1:141:B:LYS:HE2  | 5        | 0.49          |
| (1,3116) | 1:139:B:THR:HG22 | 1:141:B:LYS:HE2  | 5        | 0.49          |
| (1,3116) | 1:139:B:THR:HG23 | 1:141:B:LYS:HE2  | 5        | 0.49          |
| (1,3116) | 1:139:B:THR:HG21 | 1:141:B:LYS:HE2  | 6        | 0.49          |
| (1,3116) | 1:139:B:THR:HG22 | 1:141:B:LYS:HE2  | 6        | 0.49          |
| (1,3116) | 1:139:B:THR:HG23 | 1:141:B:LYS:HE2  | 6        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2980) | 1:125:B:GLU:HA   | 1:125:B:GLU:HG2  | 8        | 0.49          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 4        | 0.49          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 4        | 0.49          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 4        | 0.49          |
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 3        | 0.49          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE2  | 6        | 0.49          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 2        | 0.49          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 2        | 0.49          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 7        | 0.49          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 7        | 0.49          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 7        | 0.49          |
| (1,2194) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 5        | 0.49          |
| (1,2149) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 2        | 0.49          |
| (1,2149) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 2        | 0.49          |
| (1,2149) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 2        | 0.49          |
| (1,2062) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 5        | 0.49          |
| (1,2017) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB2  | 2        | 0.49          |
| (1,2017) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB2  | 2        | 0.49          |
| (1,2017) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB2  | 2        | 0.49          |
| (1,1743) | 1:148:A:VAL:H    | 1:146:A:PRO:HB3  | 6        | 0.49          |
| (1,1582) | 1:125:A:GLU:H    | 1:124:A:HIS:HB2  | 10       | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 7        | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 7        | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 7        | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 8        | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 8        | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 8        | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 10       | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 10       | 0.49          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 10       | 0.49          |
| (1,710)  | 1:126:A:GLU:HA   | 1:135:A:SER:HB2  | 5        | 0.49          |
| (1,695)  | 1:123:A:LYS:HD2  | 1:137:A:CYS:HB2  | 9        | 0.49          |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 3        | 0.49          |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 3        | 0.49          |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 3        | 0.49          |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 3        | 0.49          |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 1        | 0.49          |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 6        | 0.49          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 3        | 0.49          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 3        | 0.49          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 3        | 0.49          |
| (1,72)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB3  | 4        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB1   | 2        | 0.49          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB2   | 2        | 0.49          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB3   | 2        | 0.49          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 3        | 0.48          |
| (1,4267) | 1:167:B:ALA:H    | 1:169:B:MET:H    | 4        | 0.48          |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD3   | 8        | 0.48          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 8        | 0.48          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 4        | 0.48          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD21 | 4        | 0.48          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD22 | 4        | 0.48          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD23 | 4        | 0.48          |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 7        | 0.48          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD21 | 5        | 0.48          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD22 | 5        | 0.48          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD23 | 5        | 0.48          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 1        | 0.48          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 3        | 0.48          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 1        | 0.48          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 1        | 0.48          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 1        | 0.48          |
| (1,3274) | 1:148:B:VAL:HA   | 1:170:B:PRO:HG2  | 1        | 0.48          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 8        | 0.48          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 8        | 0.48          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 8        | 0.48          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 5        | 0.48          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 5        | 0.48          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 5        | 0.48          |
| (1,3137) | 1:141:B:LYS:HG2  | 1:142:B:TYR:HB3  | 8        | 0.48          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG22 | 5        | 0.48          |
| (1,2970) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HA   | 10       | 0.48          |
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 8        | 0.48          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 10       | 0.48          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 10       | 0.48          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 10       | 0.48          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 8        | 0.48          |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 8        | 0.48          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 8        | 0.48          |
| (1,2753) | 1:112:B:LYS:HD2  | 1:120:B:ILE:HA   | 1        | 0.48          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 7        | 0.48          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 5        | 0.48          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 6        | 0.48          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 10       | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 3        | 0.48          |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 3        | 0.48          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 3        | 0.48          |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 9        | 0.48          |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 9        | 0.48          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 9        | 0.48          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 9        | 0.48          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 10       | 0.48          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 9        | 0.48          |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 4        | 0.48          |
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 4        | 0.48          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 4        | 0.48          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 6        | 0.48          |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 10       | 0.48          |
| (1,1665) | 1:135:A:SER:H    | 1:134:A:ILE:HG21 | 9        | 0.48          |
| (1,1640) | 1:132:A:GLY:H    | 1:128:A:GLN:HG2  | 5        | 0.48          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 2        | 0.48          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 3        | 0.48          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 7        | 0.48          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 10       | 0.48          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 2        | 0.48          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 2        | 0.48          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 2        | 0.48          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 5        | 0.48          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 5        | 0.48          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 5        | 0.48          |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 7        | 0.48          |
| (1,770)  | 1:129:A:ASP:HB3  | 1:130:A:GLU:HA   | 9        | 0.48          |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 10       | 0.48          |
| (1,688)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB3  | 7        | 0.48          |
| (1,682)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HE2  | 4        | 0.48          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 3        | 0.48          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 3        | 0.48          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 3        | 0.48          |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 5        | 0.48          |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 5        | 0.48          |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 5        | 0.48          |
| (1,345)  | 1:108:A:GLU:HG2  | 1:123:A:LYS:HE2  | 3        | 0.48          |
| (1,344)  | 1:108:A:GLU:HG2  | 1:123:A:LYS:HD3  | 8        | 0.48          |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 6        | 0.48          |
| (1,282)  | 1:105:A:ALA:HA   | 1:106:A:PRO:HB2  | 10       | 0.48          |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 5        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 5        | 0.48          |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 5        | 0.48          |
| (1,99)   | 1:96:A:ARG:HB3   | 1:164:A:THR:HB   | 1        | 0.48          |
| (1,1)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HA    | 1        | 0.48          |
| (1,1)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HA    | 1        | 0.48          |
| (1,1)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HA    | 1        | 0.48          |
| (1,4255) | 1:167:B:ALA:H    | 1:95:B:TRP:HB3   | 2        | 0.47          |
| (1,3895) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB2  | 6        | 0.47          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 2        | 0.47          |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD13 | 6        | 0.47          |
| (1,3612) | 1:95:B:TRP:H     | 1:95:B:TRP:HB2   | 5        | 0.47          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 6        | 0.47          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 6        | 0.47          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 6        | 0.47          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 8        | 0.47          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 8        | 0.47          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 8        | 0.47          |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 1        | 0.47          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 7        | 0.47          |
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 7        | 0.47          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 6        | 0.47          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 6        | 0.47          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 6        | 0.47          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG21 | 1        | 0.47          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG22 | 1        | 0.47          |
| (1,2795) | 1:115:B:ASP:HB2  | 1:143:B:THR:HG23 | 1        | 0.47          |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 5        | 0.47          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 1        | 0.47          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 3        | 0.47          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 6        | 0.47          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 4        | 0.47          |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 4        | 0.47          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 4        | 0.47          |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 1        | 0.47          |
| (1,2352) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB2  | 10       | 0.47          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB1  | 5        | 0.47          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB2  | 5        | 0.47          |
| (1,1843) | 1:154:A:SER:H    | 1:167:A:ALA:HB3  | 5        | 0.47          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 7        | 0.47          |
| (1,1331) | 1:95:A:TRP:H     | 1:95:A:TRP:HB2   | 5        | 0.47          |
| (1,1302) | 1:169:A:MET:HB2  | 1:171:A:LYS:HE2  | 8        | 0.47          |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 6        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 5        | 0.47          |
| (1,930)  | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 6        | 0.47          |
| (1,930)  | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 6        | 0.47          |
| (1,930)  | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 6        | 0.47          |
| (1,930)  | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 8        | 0.47          |
| (1,930)  | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 8        | 0.47          |
| (1,930)  | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 8        | 0.47          |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 1        | 0.47          |
| (1,690)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HB2  | 10       | 0.47          |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 4        | 0.47          |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 4        | 0.47          |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 4        | 0.47          |
| (1,449)  | 1:112:A:LYS:HA   | 1:112:A:LYS:HE2  | 8        | 0.47          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 4        | 0.47          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 4        | 0.47          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 4        | 0.47          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 9        | 0.47          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 9        | 0.47          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 9        | 0.47          |
| (1,280)  | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA3  | 5        | 0.47          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 5        | 0.47          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 5        | 0.47          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 5        | 0.47          |
| (1,2)    | 1:88:A:ILE:HG21  | 1:90:A:HIS:HB3   | 8        | 0.47          |
| (1,2)    | 1:88:A:ILE:HG22  | 1:90:A:HIS:HB3   | 8        | 0.47          |
| (1,2)    | 1:88:A:ILE:HG23  | 1:90:A:HIS:HB3   | 8        | 0.47          |
| (1,4297) | 1:174:B:THR:H    | 1:171:B:LYS:HG3  | 7        | 0.46          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG21 | 10       | 0.46          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG22 | 10       | 0.46          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG23 | 10       | 0.46          |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 5        | 0.46          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 10       | 0.46          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 10       | 0.46          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 10       | 0.46          |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 6        | 0.46          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 8        | 0.46          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 8        | 0.46          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 8        | 0.46          |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG3  | 3        | 0.46          |
| (1,3694) | 1:108:B:GLU:H    | 1:106:B:PRO:HB3  | 2        | 0.46          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 9        | 0.46          |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 4        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 4        | 0.46          |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 4        | 0.46          |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 2        | 0.46          |
| (1,3378) | 1:154:B:SER:HB3  | 1:155:B:SER:HA   | 1        | 0.46          |
| (1,3303) | 1:148:B:VAL:HG21 | 1:170:B:PRO:HG2  | 1        | 0.46          |
| (1,3303) | 1:148:B:VAL:HG22 | 1:170:B:PRO:HG2  | 1        | 0.46          |
| (1,3303) | 1:148:B:VAL:HG23 | 1:170:B:PRO:HG2  | 1        | 0.46          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 6        | 0.46          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 6        | 0.46          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 6        | 0.46          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 6        | 0.46          |
| (1,3027) | 1:128:B:GLN:HA   | 1:128:B:GLN:HG3  | 1        | 0.46          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 3        | 0.46          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 3        | 0.46          |
| (1,2930) | 1:120:B:ILE:HG21 | 1:140:B:ARG:HA   | 5        | 0.46          |
| (1,2930) | 1:120:B:ILE:HG22 | 1:140:B:ARG:HA   | 5        | 0.46          |
| (1,2930) | 1:120:B:ILE:HG23 | 1:140:B:ARG:HA   | 5        | 0.46          |
| (1,2893) | 1:119:B:GLU:HA   | 1:141:B:LYS:HE3  | 9        | 0.46          |
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 8        | 0.46          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 1        | 0.46          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 3        | 0.46          |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD3  | 8        | 0.46          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 3        | 0.46          |
| (1,2563) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB2  | 9        | 0.46          |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 4        | 0.46          |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 4        | 0.46          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 4        | 0.46          |
| (1,2472) | 1:98:B:SER:HB3   | 1:99:B:LEU:HA    | 3        | 0.46          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 5        | 0.46          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 2        | 0.46          |
| (1,2352) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB2  | 9        | 0.46          |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 7        | 0.46          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 6        | 0.46          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 6        | 0.46          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 6        | 0.46          |
| (1,2194) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 10       | 0.46          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 6        | 0.46          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 6        | 0.46          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 6        | 0.46          |
| (1,2062) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 10       | 0.46          |
| (1,1916) | 1:162:A:THR:H    | 1:102:A:ASN:HB3  | 7        | 0.46          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 3        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 3        | 0.46          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 3        | 0.46          |
| (1,1664) | 1:135:A:SER:H    | 1:134:A:ILE:HG13 | 5        | 0.46          |
| (1,1612) | 1:128:A:GLN:HE22 | 1:129:A:ASP:H    | 7        | 0.46          |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 8        | 0.46          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 4        | 0.46          |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 7        | 0.46          |
| (1,1322) | 1:94:A:ARG:H     | 1:93:A:ASP:HB2   | 9        | 0.46          |
| (1,1210) | 1:160:A:GLU:HB2  | 1:162:A:THR:HB   | 7        | 0.46          |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 5        | 0.46          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG11 | 9        | 0.46          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG12 | 9        | 0.46          |
| (1,1127) | 1:155:A:SER:HB3  | 1:165:A:VAL:HG13 | 9        | 0.46          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 10       | 0.46          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 7        | 0.46          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 8        | 0.46          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 4        | 0.46          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 4        | 0.46          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 4        | 0.46          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 6        | 0.46          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 6        | 0.46          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 6        | 0.46          |
| (1,834)  | 1:139:A:THR:HG21 | 1:140:A:ARG:HG3  | 4        | 0.46          |
| (1,834)  | 1:139:A:THR:HG22 | 1:140:A:ARG:HG3  | 4        | 0.46          |
| (1,834)  | 1:139:A:THR:HG23 | 1:140:A:ARG:HG3  | 4        | 0.46          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 6        | 0.46          |
| (1,612)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HE3  | 1        | 0.46          |
| (1,528)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HB   | 4        | 0.46          |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 5        | 0.46          |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 9        | 0.46          |
| (1,107)  | 1:96:A:ARG:HG2   | 1:166:A:GLU:HG2  | 8        | 0.46          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 3        | 0.46          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 3        | 0.46          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 3        | 0.46          |
| (1,4280) | 1:169:B:MET:H    | 1:169:B:MET:HB3  | 10       | 0.45          |
| (1,4231) | 1:165:B:VAL:H    | 1:96:B:ARG:HB2   | 9        | 0.45          |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 8        | 0.45          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 7        | 0.45          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG23 | 2        | 0.45          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG22 | 7        | 0.45          |
| (1,3748) | 1:113:B:THR:H    | 1:112:B:LYS:HB2  | 8        | 0.45          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 6        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD22 | 9        | 0.45          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 6        | 0.45          |
| (1,3613) | 1:95:B:TRP:H     | 1:95:B:TRP:HE3   | 1        | 0.45          |
| (1,3612) | 1:95:B:TRP:H     | 1:95:B:TRP:HB2   | 10       | 0.45          |
| (1,3601) | 1:94:B:ARG:H     | 1:92:B:ALA:HA    | 5        | 0.45          |
| (1,3570) | 1:169:B:MET:HA   | 1:169:B:MET:HG3  | 7        | 0.45          |
| (1,3460) | 1:157:B:LEU:HD21 | 1:163:B:LEU:HB3  | 4        | 0.45          |
| (1,3460) | 1:157:B:LEU:HD22 | 1:163:B:LEU:HB3  | 4        | 0.45          |
| (1,3460) | 1:157:B:LEU:HD23 | 1:163:B:LEU:HB3  | 4        | 0.45          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 7        | 0.45          |
| (1,3420) | 1:156:B:SER:HB3  | 1:157:B:LEU:HB3  | 10       | 0.45          |
| (1,3378) | 1:154:B:SER:HB3  | 1:155:B:SER:HA   | 8        | 0.45          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 4        | 0.45          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 4        | 0.45          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 4        | 0.45          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 5        | 0.45          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 5        | 0.45          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 5        | 0.45          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 9        | 0.45          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 2        | 0.45          |
| (1,2957) | 1:122:B:GLY:HA3  | 1:137:B:CYS:HA   | 8        | 0.45          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 5        | 0.45          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 5        | 0.45          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 5        | 0.45          |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 6        | 0.45          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 6        | 0.45          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 6        | 0.45          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 5        | 0.45          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 9        | 0.45          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 10       | 0.45          |
| (1,2352) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB2  | 1        | 0.45          |
| (1,2318) | 1:94:B:ARG:HB2   | 1:96:B:ARG:HA    | 1        | 0.45          |
| (1,2314) | 1:94:B:ARG:HA    | 1:169:B:MET:HB2  | 1        | 0.45          |
| (1,2207) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 2        | 0.45          |
| (1,2207) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 2        | 0.45          |
| (1,2207) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 2        | 0.45          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 7        | 0.45          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 7        | 0.45          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 7        | 0.45          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 8        | 0.45          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 8        | 0.45          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 8        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2075) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 2        | 0.45          |
| (1,2075) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 2        | 0.45          |
| (1,2075) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 2        | 0.45          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 7        | 0.45          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 7        | 0.45          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 7        | 0.45          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 8        | 0.45          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 8        | 0.45          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 8        | 0.45          |
| (1,1924) | 1:162:A:THR:H    | 1:160:A:GLU:HB2  | 2        | 0.45          |
| (1,1767) | 1:149:A:ASP:H    | 1:170:A:PRO:HG3  | 4        | 0.45          |
| (1,1664) | 1:135:A:SER:H    | 1:134:A:ILE:HG13 | 2        | 0.45          |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 6        | 0.45          |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 7        | 0.45          |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 10       | 0.45          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 2        | 0.45          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 8        | 0.45          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 8        | 0.45          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 8        | 0.45          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 9        | 0.45          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 9        | 0.45          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 9        | 0.45          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 1        | 0.45          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 1        | 0.45          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 1        | 0.45          |
| (1,834)  | 1:139:A:THR:HG21 | 1:140:A:ARG:HG3  | 3        | 0.45          |
| (1,834)  | 1:139:A:THR:HG22 | 1:140:A:ARG:HG3  | 3        | 0.45          |
| (1,834)  | 1:139:A:THR:HG23 | 1:140:A:ARG:HG3  | 3        | 0.45          |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG21 | 10       | 0.45          |
| (1,728)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HA   | 7        | 0.45          |
| (1,723)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB2  | 5        | 0.45          |
| (1,694)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HA   | 7        | 0.45          |
| (1,690)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HB2  | 4        | 0.45          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 6        | 0.45          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 6        | 0.45          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 6        | 0.45          |
| (1,528)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HB   | 1        | 0.45          |
| (1,472)  | 1:112:A:LYS:HD2  | 1:120:A:ILE:HA   | 9        | 0.45          |
| (1,455)  | 1:112:A:LYS:HB2  | 1:112:A:LYS:HE2  | 8        | 0.45          |
| (1,434)  | 1:111:A:VAL:HG11 | 1:120:A:ILE:HG12 | 7        | 0.45          |
| (1,434)  | 1:111:A:VAL:HG12 | 1:120:A:ILE:HG12 | 7        | 0.45          |
| (1,434)  | 1:111:A:VAL:HG13 | 1:120:A:ILE:HG12 | 7        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,434)  | 1:111:A:VAL:HG11 | 1:120:A:ILE:HG12 | 9        | 0.45          |
| (1,434)  | 1:111:A:VAL:HG12 | 1:120:A:ILE:HG12 | 9        | 0.45          |
| (1,434)  | 1:111:A:VAL:HG13 | 1:120:A:ILE:HG12 | 9        | 0.45          |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 5        | 0.45          |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 9        | 0.45          |
| (1,356)  | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 2        | 0.45          |
| (1,345)  | 1:108:A:GLU:HG2  | 1:123:A:LYS:HE2  | 7        | 0.45          |
| (1,71)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB2  | 9        | 0.45          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB1   | 6        | 0.45          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB2   | 6        | 0.45          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB3   | 6        | 0.45          |
| (1,4296) | 1:173:B:ALA:H    | 1:172:B:LEU:HG   | 5        | 0.44          |
| (1,4272) | 1:169:B:MET:H    | 1:95:B:TRP:HA    | 4        | 0.44          |
| (1,4205) | 1:162:B:THR:H    | 1:160:B:GLU:HB2  | 1        | 0.44          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 3        | 0.44          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 3        | 0.44          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 3        | 0.44          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 3        | 0.44          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 8        | 0.44          |
| (1,3607) | 1:94:B:ARG:H     | 1:168:B:PRO:HA   | 9        | 0.44          |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD2  | 3        | 0.44          |
| (1,3460) | 1:157:B:LEU:HD21 | 1:163:B:LEU:HB3  | 5        | 0.44          |
| (1,3460) | 1:157:B:LEU:HD22 | 1:163:B:LEU:HB3  | 5        | 0.44          |
| (1,3460) | 1:157:B:LEU:HD23 | 1:163:B:LEU:HB3  | 5        | 0.44          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 9        | 0.44          |
| (1,3378) | 1:154:B:SER:HB3  | 1:155:B:SER:HA   | 5        | 0.44          |
| (1,3345) | 1:152:B:GLN:HB2  | 1:168:B:PRO:HD3  | 7        | 0.44          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 7        | 0.44          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 7        | 0.44          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 7        | 0.44          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 2        | 0.44          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 10       | 0.44          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 10       | 0.44          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 10       | 0.44          |
| (1,2963) | 1:123:B:LYS:HA   | 1:123:B:LYS:HE3  | 9        | 0.44          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 2        | 0.44          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 2        | 0.44          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 2        | 0.44          |
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 9        | 0.44          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 9        | 0.44          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 9        | 0.44          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 9        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 1        | 0.44          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 1        | 0.44          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 1        | 0.44          |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 6        | 0.44          |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD2  | 4        | 0.44          |
| (1,2551) | 1:101:B:VAL:HG11 | 1:102:B:ASN:HA   | 5        | 0.44          |
| (1,2551) | 1:101:B:VAL:HG12 | 1:102:B:ASN:HA   | 5        | 0.44          |
| (1,2551) | 1:101:B:VAL:HG13 | 1:102:B:ASN:HA   | 5        | 0.44          |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 3        | 0.44          |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 6        | 0.44          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 7        | 0.44          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 5        | 0.44          |
| (1,1640) | 1:132:A:GLY:H    | 1:128:A:GLN:HG2  | 4        | 0.44          |
| (1,1623) | 1:129:A:ASP:H    | 1:130:A:GLU:HG3  | 7        | 0.44          |
| (1,1482) | 1:114:A:LYS:H    | 1:115:A:ASP:HB2  | 9        | 0.44          |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD11 | 4        | 0.44          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 6        | 0.44          |
| (1,1332) | 1:95:A:TRP:H     | 1:95:A:TRP:HE3   | 10       | 0.44          |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 8        | 0.44          |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 8        | 0.44          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 8        | 0.44          |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 7        | 0.44          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 3        | 0.44          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 3        | 0.44          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 3        | 0.44          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 9        | 0.44          |
| (1,805)  | 1:134:A:ILE:HD13 | 1:135:A:SER:HB2  | 8        | 0.44          |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 9        | 0.44          |
| (1,724)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB3  | 5        | 0.44          |
| (1,722)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HA   | 9        | 0.44          |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 8        | 0.44          |
| (1,712)  | 1:126:A:GLU:HB3  | 1:133:A:TYR:HB2  | 2        | 0.44          |
| (1,682)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HE3  | 3        | 0.44          |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 6        | 0.44          |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 6        | 0.44          |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 6        | 0.44          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 7        | 0.44          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 7        | 0.44          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 7        | 0.44          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 9        | 0.44          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 9        | 0.44          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 9        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,455)  | 1:112:A:LYS:HB2  | 1:112:A:LYS:HE2  | 7        | 0.44          |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 2        | 0.44          |
| (1,257)  | 1:99:A:LEU:HD21  | 1:112:A:LYS:HG3  | 1        | 0.44          |
| (1,257)  | 1:99:A:LEU:HD22  | 1:112:A:LYS:HG3  | 1        | 0.44          |
| (1,257)  | 1:99:A:LEU:HD23  | 1:112:A:LYS:HG3  | 1        | 0.44          |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 7        | 0.44          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 3        | 0.44          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 3        | 0.44          |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD2   | 4        | 0.43          |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD3   | 7        | 0.43          |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG21 | 1        | 0.43          |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG22 | 1        | 0.43          |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG23 | 1        | 0.43          |
| (1,4197) | 1:162:B:THR:H    | 1:102:B:ASN:HB3  | 2        | 0.43          |
| (1,4084) | 1:152:B:GLN:HE21 | 1:168:B:PRO:HD2  | 1        | 0.43          |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 2        | 0.43          |
| (1,4025) | 1:148:B:VAL:H    | 1:146:B:PRO:HG2  | 8        | 0.43          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 10       | 0.43          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 10       | 0.43          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 10       | 0.43          |
| (1,3972) | 1:140:B:ARG:H    | 1:120:B:ILE:HB   | 5        | 0.43          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD1  | 1        | 0.43          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD2  | 1        | 0.43          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 5        | 0.43          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 7        | 0.43          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 7        | 0.43          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 7        | 0.43          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 5        | 0.43          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 6        | 0.43          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 6        | 0.43          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 6        | 0.43          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 8        | 0.43          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD21 | 2        | 0.43          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD22 | 2        | 0.43          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD23 | 2        | 0.43          |
| (1,3304) | 1:149:B:ASP:HA   | 1:149:B:ASP:HB3  | 1        | 0.43          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 1        | 0.43          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 1        | 0.43          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 1        | 0.43          |
| (1,3299) | 1:148:B:VAL:HG21 | 1:168:B:PRO:HD3  | 10       | 0.43          |
| (1,3299) | 1:148:B:VAL:HG22 | 1:168:B:PRO:HD3  | 10       | 0.43          |
| (1,3299) | 1:148:B:VAL:HG23 | 1:168:B:PRO:HD3  | 10       | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 1        | 0.43          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 1        | 0.43          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 1        | 0.43          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 2        | 0.43          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 2        | 0.43          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 2        | 0.43          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 7        | 0.43          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 2        | 0.43          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 6        | 0.43          |
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 2        | 0.43          |
| (1,2976) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB2  | 5        | 0.43          |
| (1,2976) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB2  | 7        | 0.43          |
| (1,2976) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB2  | 9        | 0.43          |
| (1,2975) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HA   | 9        | 0.43          |
| (1,2963) | 1:123:B:LYS:HA   | 1:123:B:LYS:HE3  | 5        | 0.43          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 8        | 0.43          |
| (1,2545) | 1:100:B:ASP:HB2  | 1:162:B:THR:HB   | 9        | 0.43          |
| (1,2513) | 1:99:B:LEU:HD11  | 1:120:B:ILE:HG12 | 2        | 0.43          |
| (1,2513) | 1:99:B:LEU:HD12  | 1:120:B:ILE:HG12 | 2        | 0.43          |
| (1,2513) | 1:99:B:LEU:HD13  | 1:120:B:ILE:HG12 | 2        | 0.43          |
| (1,2513) | 1:99:B:LEU:HD11  | 1:120:B:ILE:HG12 | 5        | 0.43          |
| (1,2513) | 1:99:B:LEU:HD12  | 1:120:B:ILE:HG12 | 5        | 0.43          |
| (1,2513) | 1:99:B:LEU:HD13  | 1:120:B:ILE:HG12 | 5        | 0.43          |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 6        | 0.43          |
| (1,2314) | 1:94:B:ARG:HA    | 1:169:B:MET:HB2  | 10       | 0.43          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 5        | 0.43          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 5        | 0.43          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 5        | 0.43          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 5        | 0.43          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 5        | 0.43          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 5        | 0.43          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 3        | 0.43          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 8        | 0.43          |
| (1,1799) | 1:152:A:GLN:HE21 | 1:152:A:GLN:HB3  | 3        | 0.43          |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 9        | 0.43          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 8        | 0.43          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 1        | 0.43          |
| (1,1288) | 1:169:A:MET:HA   | 1:169:A:MET:HG2  | 6        | 0.43          |
| (1,1260) | 1:166:A:GLU:HG3  | 1:168:A:PRO:HD3  | 1        | 0.43          |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 9        | 0.43          |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 9        | 0.43          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 9        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 6        | 0.43          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 6        | 0.43          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 6        | 0.43          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 6        | 0.43          |
| (1,1085) | 1:153:A:VAL:HG21 | 1:155:A:SER:HB3  | 1        | 0.43          |
| (1,1085) | 1:153:A:VAL:HG22 | 1:155:A:SER:HB3  | 1        | 0.43          |
| (1,1085) | 1:153:A:VAL:HG23 | 1:155:A:SER:HB3  | 1        | 0.43          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 5        | 0.43          |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 1        | 0.43          |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG23 | 8        | 0.43          |
| (1,694)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HA   | 2        | 0.43          |
| (1,694)  | 1:123:A:LYS:HD2  | 1:137:A:CYS:HA   | 6        | 0.43          |
| (1,682)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HE3  | 8        | 0.43          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 4        | 0.43          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 4        | 0.43          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 4        | 0.43          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 8        | 0.43          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 8        | 0.43          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 8        | 0.43          |
| (1,509)  | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 8        | 0.43          |
| (1,418)  | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 6        | 0.43          |
| (1,418)  | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 7        | 0.43          |
| (1,405)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HD3  | 2        | 0.43          |
| (1,405)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HD3  | 2        | 0.43          |
| (1,405)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HD3  | 2        | 0.43          |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 7        | 0.43          |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 7        | 0.43          |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 7        | 0.43          |
| (1,370)  | 1:109:A:LEU:HD11 | 1:122:A:GLY:HA3  | 5        | 0.43          |
| (1,370)  | 1:109:A:LEU:HD12 | 1:122:A:GLY:HA3  | 5        | 0.43          |
| (1,370)  | 1:109:A:LEU:HD13 | 1:122:A:GLY:HA3  | 5        | 0.43          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 1        | 0.43          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 1        | 0.43          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 1        | 0.43          |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD21 | 1        | 0.43          |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD22 | 1        | 0.43          |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD23 | 1        | 0.43          |
| (1,247)  | 1:99:A:LEU:HD21  | 1:140:A:ARG:HG3  | 3        | 0.43          |
| (1,247)  | 1:99:A:LEU:HD22  | 1:140:A:ARG:HG3  | 3        | 0.43          |
| (1,247)  | 1:99:A:LEU:HD23  | 1:140:A:ARG:HG3  | 3        | 0.43          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 8        | 0.43          |
| (1,71)   | 1:95:A:TRP:HB2   | 1:168:A:PRO:HB2  | 5        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,71)   | 1:95:A:TRP:HB2   | 1:168:A:PRO:HB2  | 8        | 0.43          |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 9        | 0.43          |
| (1,7)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HA    | 8        | 0.43          |
| (1,4197) | 1:162:B:THR:H    | 1:102:B:ASN:HB3  | 8        | 0.42          |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 6        | 0.42          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 3        | 0.42          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 3        | 0.42          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 3        | 0.42          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 2        | 0.42          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 2        | 0.42          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 2        | 0.42          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 4        | 0.42          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 4        | 0.42          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 4        | 0.42          |
| (1,3904) | 1:129:B:ASP:H    | 1:130:B:GLU:HG3  | 6        | 0.42          |
| (1,3904) | 1:129:B:ASP:H    | 1:130:B:GLU:HG3  | 9        | 0.42          |
| (1,3895) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB2  | 7        | 0.42          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 10       | 0.42          |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD11 | 2        | 0.42          |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD21 | 7        | 0.42          |
| (1,3491) | 1:160:B:GLU:HB2  | 1:162:B:THR:HB   | 2        | 0.42          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 3        | 0.42          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 3        | 0.42          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 3        | 0.42          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 4        | 0.42          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 4        | 0.42          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 4        | 0.42          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 9        | 0.42          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 9        | 0.42          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 9        | 0.42          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 3        | 0.42          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 9        | 0.42          |
| (1,3013) | 1:126:B:GLU:HG3  | 1:134:B:ILE:HG22 | 10       | 0.42          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 4        | 0.42          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 1        | 0.42          |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 10       | 0.42          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 3        | 0.42          |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 3        | 0.42          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 3        | 0.42          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 3        | 0.42          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 8        | 0.42          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 6        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD11 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD12 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD13 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD11 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD12 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD13 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD11 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD12 | 4        | 0.42          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD13 | 4        | 0.42          |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 5        | 0.42          |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 5        | 0.42          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 5        | 0.42          |
| (1,2468) | 1:98:B:SER:HB2   | 1:164:B:THR:HB   | 8        | 0.42          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 6        | 0.42          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 7        | 0.42          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 2        | 0.42          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 2        | 0.42          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 2        | 0.42          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 4        | 0.42          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 4        | 0.42          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 4        | 0.42          |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 2        | 0.42          |
| (1,2157) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 5        | 0.42          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 2        | 0.42          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 2        | 0.42          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 2        | 0.42          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 4        | 0.42          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 4        | 0.42          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 4        | 0.42          |
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 2        | 0.42          |
| (1,2025) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 5        | 0.42          |
| (1,2009) | 1:171:A:LYS:H    | 1:171:A:LYS:HB2  | 9        | 0.42          |
| (1,2008) | 1:171:A:LYS:H    | 1:171:A:LYS:HA   | 9        | 0.42          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD3   | 3        | 0.42          |
| (1,1974) | 1:167:A:ALA:H    | 1:95:A:TRP:HB3   | 10       | 0.42          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 10       | 0.42          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 5        | 0.42          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 5        | 0.42          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 5        | 0.42          |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG2  | 8        | 0.42          |
| (1,1623) | 1:129:A:ASP:H    | 1:130:A:GLU:HG3  | 2        | 0.42          |
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 4        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1552) | 1:121:A:THR:H    | 1:120:A:ILE:HG12 | 10       | 0.42          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 9        | 0.42          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 5        | 0.42          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 5        | 0.42          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 5        | 0.42          |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 3        | 0.42          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 1        | 0.42          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 1        | 0.42          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 1        | 0.42          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 9        | 0.42          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 9        | 0.42          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 9        | 0.42          |
| (1,930)  | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 4        | 0.42          |
| (1,930)  | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 4        | 0.42          |
| (1,930)  | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 4        | 0.42          |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 6        | 0.42          |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 6        | 0.42          |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 6        | 0.42          |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 7        | 0.42          |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 7        | 0.42          |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 7        | 0.42          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 3        | 0.42          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 3        | 0.42          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 3        | 0.42          |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 1        | 0.42          |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 10       | 0.42          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 3        | 0.42          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 5        | 0.42          |
| (1,722)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HA   | 3        | 0.42          |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 5        | 0.42          |
| (1,695)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HB2  | 2        | 0.42          |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 10       | 0.42          |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 10       | 0.42          |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 10       | 0.42          |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 4        | 0.42          |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 4        | 0.42          |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 4        | 0.42          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 7        | 0.42          |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 9        | 0.42          |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 9        | 0.42          |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 9        | 0.42          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 2        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,71)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB2  | 6        | 0.42          |
| (1,49)   | 1:94:A:ARG:HD3   | 1:168:A:PRO:HA   | 8        | 0.42          |
| (1,41)   | 1:94:A:ARG:HB3   | 1:167:A:ALA:HA   | 4        | 0.42          |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG21  | 1        | 0.42          |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG22  | 1        | 0.42          |
| (1,6)    | 1:90:A:HIS:HA    | 1:91:A:THR:HG23  | 1        | 0.42          |
| (1,4285) | 1:171:B:LYS:H    | 1:169:B:MET:HA   | 6        | 0.41          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG21 | 10       | 0.41          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE1  | 8        | 0.41          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE2  | 8        | 0.41          |
| (1,3689) | 1:107:B:ASP:H    | 1:157:B:LEU:HD13 | 3        | 0.41          |
| (1,3603) | 1:94:B:ARG:H     | 1:93:B:ASP:HB2   | 7        | 0.41          |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD3  | 8        | 0.41          |
| (1,3255) | 1:147:B:GLY:HA2  | 1:148:B:VAL:HG11 | 9        | 0.41          |
| (1,3255) | 1:147:B:GLY:HA2  | 1:148:B:VAL:HG12 | 9        | 0.41          |
| (1,3255) | 1:147:B:GLY:HA2  | 1:148:B:VAL:HG13 | 9        | 0.41          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 8        | 0.41          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 8        | 0.41          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 8        | 0.41          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 9        | 0.41          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 9        | 0.41          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 9        | 0.41          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 6        | 0.41          |
| (1,3092) | 1:136:B:ARG:HA   | 1:136:B:ARG:HG2  | 10       | 0.41          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 9        | 0.41          |
| (1,3002) | 1:126:B:GLU:HG2  | 1:134:B:ILE:HG23 | 4        | 0.41          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 2        | 0.41          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 2        | 0.41          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 2        | 0.41          |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 8        | 0.41          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 6        | 0.41          |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 2        | 0.41          |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 2        | 0.41          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 2        | 0.41          |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 2        | 0.41          |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 2        | 0.41          |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 2        | 0.41          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG21  | 5        | 0.41          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG22  | 5        | 0.41          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG23  | 5        | 0.41          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 3        | 0.41          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB1  | 9        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB2  | 9        | 0.41          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB3  | 9        | 0.41          |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 2        | 0.41          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 10       | 0.41          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 10       | 0.41          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 10       | 0.41          |
| (1,2213) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 10       | 0.41          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 6        | 0.41          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 6        | 0.41          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 6        | 0.41          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 10       | 0.41          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 10       | 0.41          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 10       | 0.41          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 10       | 0.41          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 10       | 0.41          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 10       | 0.41          |
| (1,2081) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 10       | 0.41          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 6        | 0.41          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 6        | 0.41          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 6        | 0.41          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 10       | 0.41          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 10       | 0.41          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 10       | 0.41          |
| (1,2008) | 1:171:A:LYS:H    | 1:171:A:LYS:HA   | 10       | 0.41          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 8        | 0.41          |
| (1,1812) | 1:152:A:GLN:HE22 | 1:168:A:PRO:HD3  | 1        | 0.41          |
| (1,1756) | 1:148:A:VAL:H    | 1:170:A:PRO:HG3  | 2        | 0.41          |
| (1,1408) | 1:107:A:ASP:H    | 1:157:A:LEU:HD12 | 3        | 0.41          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD21 | 3        | 0.41          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD22 | 3        | 0.41          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD23 | 3        | 0.41          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD21 | 10       | 0.41          |
| (1,1332) | 1:95:A:TRP:H     | 1:95:A:TRP:HE3   | 7        | 0.41          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 5        | 0.41          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 5        | 0.41          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 5        | 0.41          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 5        | 0.41          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 5        | 0.41          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 5        | 0.41          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 3        | 0.41          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 3        | 0.41          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 3        | 0.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,974) | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 8        | 0.41          |
| (1,974) | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 8        | 0.41          |
| (1,974) | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 8        | 0.41          |
| (1,930) | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 2        | 0.41          |
| (1,930) | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 2        | 0.41          |
| (1,930) | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 2        | 0.41          |
| (1,930) | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 3        | 0.41          |
| (1,930) | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 3        | 0.41          |
| (1,930) | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 3        | 0.41          |
| (1,930) | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 5        | 0.41          |
| (1,930) | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 5        | 0.41          |
| (1,930) | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 5        | 0.41          |
| (1,930) | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 7        | 0.41          |
| (1,930) | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 7        | 0.41          |
| (1,930) | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 7        | 0.41          |
| (1,930) | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 9        | 0.41          |
| (1,930) | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 9        | 0.41          |
| (1,930) | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 9        | 0.41          |
| (1,928) | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 3        | 0.41          |
| (1,928) | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 3        | 0.41          |
| (1,928) | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 3        | 0.41          |
| (1,845) | 1:141:A:LYS:HA   | 1:141:A:LYS:HD3  | 7        | 0.41          |
| (1,705) | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 3        | 0.41          |
| (1,695) | 1:123:A:LYS:HD2  | 1:137:A:CYS:HB2  | 6        | 0.41          |
| (1,694) | 1:123:A:LYS:HD3  | 1:137:A:CYS:HA   | 5        | 0.41          |
| (1,689) | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 3        | 0.41          |
| (1,509) | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 5        | 0.41          |
| (1,383) | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 5        | 0.41          |
| (1,383) | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 5        | 0.41          |
| (1,383) | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 5        | 0.41          |
| (1,362) | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 6        | 0.41          |
| (1,362) | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 10       | 0.41          |
| (1,356) | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 6        | 0.41          |
| (1,356) | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 9        | 0.41          |
| (1,356) | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 10       | 0.41          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 8        | 0.41          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 8        | 0.41          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 8        | 0.41          |
| (1,270) | 1:101:A:VAL:HG11 | 1:102:A:ASN:HA   | 8        | 0.41          |
| (1,270) | 1:101:A:VAL:HG12 | 1:102:A:ASN:HA   | 8        | 0.41          |
| (1,270) | 1:101:A:VAL:HG13 | 1:102:A:ASN:HA   | 8        | 0.41          |
| (1,96)  | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 6        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4262) | 1:167:B:ALA:H    | 1:166:B:GLU:HB2  | 4        | 0.4           |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 2        | 0.4           |
| (1,4047) | 1:149:B:ASP:H    | 1:169:B:MET:HG3  | 7        | 0.4           |
| (1,4037) | 1:148:B:VAL:H    | 1:170:B:PRO:HG3  | 6        | 0.4           |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 7        | 0.4           |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 7        | 0.4           |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 7        | 0.4           |
| (1,3902) | 1:129:B:ASP:H    | 1:129:B:ASP:HB2  | 3        | 0.4           |
| (1,3847) | 1:123:B:LYS:H    | 1:109:B:LEU:HB2  | 6        | 0.4           |
| (1,3806) | 1:119:B:GLU:H    | 1:114:B:LYS:HB3  | 10       | 0.4           |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 8        | 0.4           |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 8        | 0.4           |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 8        | 0.4           |
| (1,3612) | 1:95:B:TRP:H     | 1:95:B:TRP:HB2   | 2        | 0.4           |
| (1,3612) | 1:95:B:TRP:H     | 1:95:B:TRP:HB2   | 3        | 0.4           |
| (1,3601) | 1:94:B:ARG:H     | 1:92:B:ALA:HA    | 1        | 0.4           |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 8        | 0.4           |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 4        | 0.4           |
| (1,3460) | 1:157:B:LEU:HD21 | 1:163:B:LEU:HB3  | 2        | 0.4           |
| (1,3460) | 1:157:B:LEU:HD22 | 1:163:B:LEU:HB3  | 2        | 0.4           |
| (1,3460) | 1:157:B:LEU:HD23 | 1:163:B:LEU:HB3  | 2        | 0.4           |
| (1,3303) | 1:148:B:VAL:HG21 | 1:170:B:PRO:HG2  | 3        | 0.4           |
| (1,3303) | 1:148:B:VAL:HG22 | 1:170:B:PRO:HG2  | 3        | 0.4           |
| (1,3303) | 1:148:B:VAL:HG23 | 1:170:B:PRO:HG2  | 3        | 0.4           |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 10       | 0.4           |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 10       | 0.4           |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 10       | 0.4           |
| (1,3126) | 1:141:B:LYS:HA   | 1:141:B:LYS:HD3  | 9        | 0.4           |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 2        | 0.4           |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 2        | 0.4           |
| (1,2976) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HB2  | 8        | 0.4           |
| (1,2975) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HA   | 5        | 0.4           |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE2  | 10       | 0.4           |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 2        | 0.4           |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 4        | 0.4           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 2        | 0.4           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 2        | 0.4           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 2        | 0.4           |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG21 | 10       | 0.4           |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG22 | 10       | 0.4           |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG23 | 10       | 0.4           |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 6        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 6        | 0.4           |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 6        | 0.4           |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 5        | 0.4           |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 5        | 0.4           |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 5        | 0.4           |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 5        | 0.4           |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 5        | 0.4           |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 5        | 0.4           |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 7        | 0.4           |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 7        | 0.4           |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 7        | 0.4           |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB1  | 7        | 0.4           |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB2  | 7        | 0.4           |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB3  | 7        | 0.4           |
| (1,2328) | 1:94:B:ARG:HG3   | 1:168:B:PRO:HB3  | 7        | 0.4           |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 1        | 0.4           |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 9        | 0.4           |
| (1,1950) | 1:165:A:VAL:H    | 1:96:A:ARG:HB2   | 5        | 0.4           |
| (1,1924) | 1:162:A:THR:H    | 1:160:A:GLU:HB2  | 4        | 0.4           |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 4        | 0.4           |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 4        | 0.4           |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 2        | 0.4           |
| (1,1331) | 1:95:A:TRP:H     | 1:95:A:TRP:HB2   | 3        | 0.4           |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 1        | 0.4           |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 1        | 0.4           |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 1        | 0.4           |
| (1,1114) | 1:155:A:SER:HB2  | 1:163:A:LEU:HA   | 6        | 0.4           |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 4        | 0.4           |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 4        | 0.4           |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 4        | 0.4           |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 1        | 0.4           |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 1        | 0.4           |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 1        | 0.4           |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 8        | 0.4           |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 8        | 0.4           |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 8        | 0.4           |
| (1,917)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA2  | 10       | 0.4           |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 5        | 0.4           |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 5        | 0.4           |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 5        | 0.4           |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 1        | 0.4           |
| (1,455)  | 1:112:A:LYS:HB2  | 1:112:A:LYS:HE2  | 3        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,449)  | 1:112:A:LYS:HA   | 1:112:A:LYS:HE2  | 3        | 0.4           |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 3        | 0.4           |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 3        | 0.4           |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 3        | 0.4           |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 8        | 0.4           |
| (1,356)  | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 4        | 0.4           |
| (1,356)  | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 8        | 0.4           |
| (1,348)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HE3  | 6        | 0.4           |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 10       | 0.4           |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 10       | 0.4           |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 10       | 0.4           |
| (1,99)   | 1:96:A:ARG:HB3   | 1:164:A:THR:HB   | 5        | 0.4           |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 1        | 0.4           |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 9        | 0.4           |
| (1,50)   | 1:94:A:ARG:HD2   | 1:168:A:PRO:HB2  | 8        | 0.4           |
| (1,16)   | 1:93:A:ASP:HA    | 1:94:A:ARG:HD2   | 6        | 0.4           |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 4        | 0.39          |
| (1,4037) | 1:148:B:VAL:H    | 1:170:B:PRO:HG3  | 9        | 0.39          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG22 | 6        | 0.39          |
| (1,3910) | 1:129:B:ASP:H    | 1:133:B:TYR:HB2  | 4        | 0.39          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 4        | 0.39          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 4        | 0.39          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 9        | 0.39          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 9        | 0.39          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 9        | 0.39          |
| (1,3612) | 1:95:B:TRP:H     | 1:95:B:TRP:HB2   | 4        | 0.39          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 8        | 0.39          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 5        | 0.39          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 5        | 0.39          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 5        | 0.39          |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 5        | 0.39          |
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 5        | 0.39          |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 5        | 0.39          |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 3        | 0.39          |
| (1,3395) | 1:155:B:SER:HB2  | 1:163:B:LEU:HA   | 6        | 0.39          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG21 | 6        | 0.39          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG22 | 6        | 0.39          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG23 | 6        | 0.39          |
| (1,3128) | 1:141:B:LYS:HA   | 1:141:B:LYS:HE3  | 9        | 0.39          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 4        | 0.39          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 2        | 0.39          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 2        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 6        | 0.39          |
| (1,2935) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HD2  | 6        | 0.39          |
| (1,2935) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HD2  | 6        | 0.39          |
| (1,2935) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HD2  | 6        | 0.39          |
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 4        | 0.39          |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE2  | 6        | 0.39          |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE3  | 3        | 0.39          |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE3  | 3        | 0.39          |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE3  | 3        | 0.39          |
| (1,2666) | 1:109:B:LEU:HD21 | 1:161:B:GLY:HA3  | 3        | 0.39          |
| (1,2666) | 1:109:B:LEU:HD22 | 1:161:B:GLY:HA3  | 3        | 0.39          |
| (1,2666) | 1:109:B:LEU:HD23 | 1:161:B:GLY:HA3  | 3        | 0.39          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 1        | 0.39          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 9        | 0.39          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD21 | 1        | 0.39          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD22 | 1        | 0.39          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD23 | 1        | 0.39          |
| (1,2332) | 1:95:B:TRP:HA    | 1:95:B:TRP:HB2   | 6        | 0.39          |
| (1,2299) | 1:93:B:ASP:HB2   | 1:94:B:ARG:HA    | 10       | 0.39          |
| (1,2288) | 1:90:B:HIS:HB2   | 1:91:B:THR:HA    | 2        | 0.39          |
| (1,2002) | 1:169:A:MET:H    | 1:171:A:LYS:HE3  | 1        | 0.39          |
| (1,1899) | 1:160:A:GLU:H    | 1:160:A:GLU:HG3  | 3        | 0.39          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 5        | 0.39          |
| (1,1816) | 1:153:A:VAL:H    | 1:149:A:ASP:HB2  | 3        | 0.39          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD22 | 1        | 0.39          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 9        | 0.39          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 2        | 0.39          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 2        | 0.39          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 2        | 0.39          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 10       | 0.39          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 10       | 0.39          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 10       | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 5        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 5        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 5        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 7        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 7        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 7        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 9        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 9        | 0.39          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 9        | 0.39          |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 4        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 4        | 0.39          |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 4        | 0.39          |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 4        | 0.39          |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 7        | 0.39          |
| (1,418)  | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 9        | 0.39          |
| (1,406)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HE3  | 7        | 0.39          |
| (1,406)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HE3  | 7        | 0.39          |
| (1,406)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HE3  | 7        | 0.39          |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 2        | 0.39          |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 2        | 0.39          |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 2        | 0.39          |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 4        | 0.39          |
| (1,356)  | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 5        | 0.39          |
| (1,264)  | 1:100:A:ASP:HB2  | 1:162:A:THR:HB   | 2        | 0.39          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 3        | 0.39          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 10       | 0.39          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 10       | 0.39          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 10       | 0.39          |
| (1,71)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB2  | 2        | 0.39          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 9        | 0.39          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 9        | 0.39          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 9        | 0.39          |
| (1,17)   | 1:93:A:ASP:HA    | 1:169:A:MET:HG2  | 2        | 0.39          |
| (1,4289) | 1:171:B:LYS:H    | 1:171:B:LYS:HA   | 5        | 0.38          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 3        | 0.38          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 10       | 0.38          |
| (1,4095) | 1:152:B:GLN:HE22 | 1:170:B:PRO:HD3  | 7        | 0.38          |
| (1,3848) | 1:123:B:LYS:H    | 1:109:B:LEU:HG   | 8        | 0.38          |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 3        | 0.38          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 10       | 0.38          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 3        | 0.38          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 3        | 0.38          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 3        | 0.38          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 4        | 0.38          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD21 | 2        | 0.38          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD22 | 2        | 0.38          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD23 | 2        | 0.38          |
| (1,3378) | 1:154:B:SER:HB3  | 1:155:B:SER:HA   | 4        | 0.38          |
| (1,3345) | 1:152:B:GLN:HB2  | 1:168:B:PRO:HD3  | 8        | 0.38          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG11 | 9        | 0.38          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG12 | 9        | 0.38          |
| (1,3193) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG13 | 9        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 8        | 0.38          |
| (1,3107) | 1:139:B:THR:HA   | 1:140:B:ARG:HB2  | 5        | 0.38          |
| (1,3092) | 1:136:B:ARG:HA   | 1:136:B:ARG:HG2  | 8        | 0.38          |
| (1,3014) | 1:126:B:GLU:HG3  | 1:135:B:SER:HB3  | 6        | 0.38          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 1        | 0.38          |
| (1,2976) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HB2  | 2        | 0.38          |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 1        | 0.38          |
| (1,2651) | 1:109:B:LEU:HD11 | 1:122:B:GLY:HA3  | 9        | 0.38          |
| (1,2651) | 1:109:B:LEU:HD12 | 1:122:B:GLY:HA3  | 9        | 0.38          |
| (1,2651) | 1:109:B:LEU:HD13 | 1:122:B:GLY:HA3  | 9        | 0.38          |
| (1,2626) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HE2  | 5        | 0.38          |
| (1,2617) | 1:108:B:GLU:HA   | 1:108:B:GLU:HG2  | 9        | 0.38          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 2        | 0.38          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 5        | 0.38          |
| (1,2568) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB3  | 10       | 0.38          |
| (1,2529) | 1:99:B:LEU:HD21  | 1:140:B:ARG:HD2  | 2        | 0.38          |
| (1,2529) | 1:99:B:LEU:HD22  | 1:140:B:ARG:HD2  | 2        | 0.38          |
| (1,2529) | 1:99:B:LEU:HD23  | 1:140:B:ARG:HD2  | 2        | 0.38          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 9        | 0.38          |
| (1,2331) | 1:94:B:ARG:HD3   | 1:168:B:PRO:HB2  | 8        | 0.38          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 10       | 0.38          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 1        | 0.38          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 1        | 0.38          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 1        | 0.38          |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 3        | 0.38          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 1        | 0.38          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 1        | 0.38          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 1        | 0.38          |
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 3        | 0.38          |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 1        | 0.38          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 2        | 0.38          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD3   | 9        | 0.38          |
| (1,1799) | 1:152:A:GLN:HE21 | 1:152:A:GLN:HB3  | 8        | 0.38          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 6        | 0.38          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 6        | 0.38          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 6        | 0.38          |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 5        | 0.38          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 9        | 0.38          |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD13 | 5        | 0.38          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD22 | 5        | 0.38          |
| (1,1326) | 1:94:A:ARG:H     | 1:168:A:PRO:HA   | 1        | 0.38          |
| (1,1288) | 1:169:A:MET:HA   | 1:169:A:MET:HG2  | 7        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1197) | 1:158:A:SER:HB3  | 1:159:A:PRO:HD3  | 5        | 0.38          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 2        | 0.38          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 2        | 0.38          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 2        | 0.38          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 4        | 0.38          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 4        | 0.38          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 4        | 0.38          |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 5        | 0.38          |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 5        | 0.38          |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 5        | 0.38          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD1  | 8        | 0.38          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD2  | 8        | 0.38          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD1  | 8        | 0.38          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD2  | 8        | 0.38          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD1  | 8        | 0.38          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD2  | 8        | 0.38          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 6        | 0.38          |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 4        | 0.38          |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 2        | 0.38          |
| (1,509)  | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 4        | 0.38          |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 3        | 0.38          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 3        | 0.38          |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 3        | 0.38          |
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 4        | 0.38          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 4        | 0.38          |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 4        | 0.38          |
| (1,383)  | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 4        | 0.38          |
| (1,383)  | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 4        | 0.38          |
| (1,383)  | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 4        | 0.38          |
| (1,362)  | 1:109:A:LEU:HB3  | 1:121:A:THR:HB   | 1        | 0.38          |
| (1,356)  | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 3        | 0.38          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 1        | 0.38          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 2        | 0.38          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 8        | 0.38          |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD21 | 5        | 0.38          |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD22 | 5        | 0.38          |
| (1,277)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD23 | 5        | 0.38          |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 3        | 0.38          |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 3        | 0.38          |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 3        | 0.38          |
| (1,256)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 1        | 0.38          |
| (1,256)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 1        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,256)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 1        | 0.38          |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 7        | 0.38          |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG21  | 8        | 0.38          |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG22  | 8        | 0.38          |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG23  | 8        | 0.38          |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 6        | 0.38          |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD2   | 2        | 0.37          |
| (1,4095) | 1:152:B:GLN:HE22 | 1:170:B:PRO:HD3  | 4        | 0.37          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 5        | 0.37          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 5        | 0.37          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 5        | 0.37          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE1  | 5        | 0.37          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE2  | 5        | 0.37          |
| (1,3902) | 1:129:B:ASP:H    | 1:129:B:ASP:HB2  | 7        | 0.37          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 5        | 0.37          |
| (1,3474) | 1:158:B:SER:HB3  | 1:160:B:GLU:HB3  | 8        | 0.37          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 2        | 0.37          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 10       | 0.37          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 9        | 0.37          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 6        | 0.37          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 6        | 0.37          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 6        | 0.37          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 8        | 0.37          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 8        | 0.37          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 8        | 0.37          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 3        | 0.37          |
| (1,3137) | 1:141:B:LYS:HG2  | 1:142:B:TYR:HB3  | 1        | 0.37          |
| (1,3137) | 1:141:B:LYS:HG2  | 1:142:B:TYR:HB3  | 2        | 0.37          |
| (1,3122) | 1:140:B:ARG:HG2  | 1:142:B:TYR:HE1  | 2        | 0.37          |
| (1,3122) | 1:140:B:ARG:HG2  | 1:142:B:TYR:HE2  | 2        | 0.37          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 3        | 0.37          |
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 5        | 0.37          |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 8        | 0.37          |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 1        | 0.37          |
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 1        | 0.37          |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 1        | 0.37          |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE2  | 10       | 0.37          |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 8        | 0.37          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 8        | 0.37          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 8        | 0.37          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 10       | 0.37          |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 7        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 7        | 0.37          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 7        | 0.37          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 2        | 0.37          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 2        | 0.37          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 2        | 0.37          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 4        | 0.37          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 10       | 0.37          |
| (1,2385) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HA   | 10       | 0.37          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 9        | 0.37          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 9        | 0.37          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 9        | 0.37          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG21 | 9        | 0.37          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG22 | 9        | 0.37          |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG23 | 9        | 0.37          |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 10       | 0.37          |
| (1,2169) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 10       | 0.37          |
| (1,2037) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 10       | 0.37          |
| (1,1998) | 1:169:A:MET:H    | 1:169:A:MET:HB2  | 10       | 0.37          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 7        | 0.37          |
| (1,1940) | 1:164:A:THR:H    | 1:162:A:THR:HG21 | 2        | 0.37          |
| (1,1940) | 1:164:A:THR:H    | 1:162:A:THR:HG22 | 2        | 0.37          |
| (1,1940) | 1:164:A:THR:H    | 1:162:A:THR:HG23 | 2        | 0.37          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 4        | 0.37          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 10       | 0.37          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 7        | 0.37          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 7        | 0.37          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 7        | 0.37          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 8        | 0.37          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 8        | 0.37          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 8        | 0.37          |
| (1,1197) | 1:158:A:SER:HB3  | 1:159:A:PRO:HD3  | 1        | 0.37          |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 7        | 0.37          |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 1        | 0.37          |
| (1,930)  | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 1        | 0.37          |
| (1,930)  | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 1        | 0.37          |
| (1,930)  | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 1        | 0.37          |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 2        | 0.37          |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 2        | 0.37          |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 2        | 0.37          |
| (1,928)  | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 9        | 0.37          |
| (1,928)  | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 9        | 0.37          |
| (1,928)  | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 9        | 0.37          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,928) | 1:144:A:LEU:HD11 | 1:145:A:PRO:HB3  | 10       | 0.37          |
| (1,928) | 1:144:A:LEU:HD12 | 1:145:A:PRO:HB3  | 10       | 0.37          |
| (1,928) | 1:144:A:LEU:HD13 | 1:145:A:PRO:HB3  | 10       | 0.37          |
| (1,856) | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 6        | 0.37          |
| (1,777) | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 5        | 0.37          |
| (1,731) | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE1  | 5        | 0.37          |
| (1,731) | 1:126:A:GLU:HG3  | 1:133:A:TYR:HE2  | 5        | 0.37          |
| (1,728) | 1:126:A:GLU:HG3  | 1:133:A:TYR:HA   | 9        | 0.37          |
| (1,705) | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 9        | 0.37          |
| (1,652) | 1:120:A:ILE:HD11 | 1:140:A:ARG:HB2  | 10       | 0.37          |
| (1,652) | 1:120:A:ILE:HD12 | 1:140:A:ARG:HB2  | 10       | 0.37          |
| (1,652) | 1:120:A:ILE:HD13 | 1:140:A:ARG:HB2  | 10       | 0.37          |
| (1,639) | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 1        | 0.37          |
| (1,639) | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 5        | 0.37          |
| (1,589) | 1:118:A:VAL:HG11 | 1:148:A:VAL:HB   | 6        | 0.37          |
| (1,589) | 1:118:A:VAL:HG12 | 1:148:A:VAL:HB   | 6        | 0.37          |
| (1,589) | 1:118:A:VAL:HG13 | 1:148:A:VAL:HB   | 6        | 0.37          |
| (1,383) | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 8        | 0.37          |
| (1,383) | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 8        | 0.37          |
| (1,383) | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 8        | 0.37          |
| (1,359) | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 5        | 0.37          |
| (1,356) | 1:109:A:LEU:HA   | 1:122:A:GLY:HA2  | 7        | 0.37          |
| (1,320) | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 4        | 0.37          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG21 | 9        | 0.37          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG22 | 9        | 0.37          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG23 | 9        | 0.37          |
| (1,258) | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 8        | 0.37          |
| (1,258) | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 8        | 0.37          |
| (1,258) | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 8        | 0.37          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 7        | 0.37          |
| (1,240) | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 7        | 0.37          |
| (1,232) | 1:99:A:LEU:HD11  | 1:120:A:ILE:HG12 | 4        | 0.37          |
| (1,232) | 1:99:A:LEU:HD12  | 1:120:A:ILE:HG12 | 4        | 0.37          |
| (1,232) | 1:99:A:LEU:HD13  | 1:120:A:ILE:HG12 | 4        | 0.37          |
| (1,184) | 1:98:A:SER:HB2   | 1:162:A:THR:HG21 | 3        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,184)  | 1:98:A:SER:HB2   | 1:162:A:THR:HG22 | 3        | 0.37          |
| (1,184)  | 1:98:A:SER:HB2   | 1:162:A:THR:HG23 | 3        | 0.37          |
| (1,166)  | 1:97:A:VAL:HG21  | 1:118:A:VAL:HB   | 1        | 0.37          |
| (1,166)  | 1:97:A:VAL:HG22  | 1:118:A:VAL:HB   | 1        | 0.37          |
| (1,166)  | 1:97:A:VAL:HG23  | 1:118:A:VAL:HB   | 1        | 0.37          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 7        | 0.37          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 7        | 0.37          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 7        | 0.37          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 6        | 0.37          |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 2        | 0.37          |
| (1,33)   | 1:94:A:ARG:HA    | 1:169:A:MET:HB2  | 1        | 0.37          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 4        | 0.37          |
| (1,4293) | 1:172:B:LEU:H    | 1:171:B:LYS:HA   | 2        | 0.36          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB1  | 7        | 0.36          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB2  | 7        | 0.36          |
| (1,4274) | 1:169:B:MET:H    | 1:167:B:ALA:HB3  | 7        | 0.36          |
| (1,4191) | 1:161:B:GLY:H    | 1:160:B:GLU:HG3  | 9        | 0.36          |
| (1,3946) | 1:135:B:SER:H    | 1:134:B:ILE:HG22 | 8        | 0.36          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 6        | 0.36          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 9        | 0.36          |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD22 | 1        | 0.36          |
| (1,3492) | 1:160:B:GLU:HG2  | 1:162:B:THR:HB   | 9        | 0.36          |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 9        | 0.36          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 1        | 0.36          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 2        | 0.36          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 6        | 0.36          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 6        | 0.36          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 6        | 0.36          |
| (1,3139) | 1:141:B:LYS:HG3  | 1:141:B:LYS:HE2  | 10       | 0.36          |
| (1,3060) | 1:131:B:HIS:HA   | 1:131:B:HIS:HE1  | 9        | 0.36          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 6        | 0.36          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 7        | 0.36          |
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 3        | 0.36          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 6        | 0.36          |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 6        | 0.36          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 6        | 0.36          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 3        | 0.36          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 3        | 0.36          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 3        | 0.36          |
| (1,2738) | 1:112:B:LYS:HB2  | 1:120:B:ILE:HA   | 8        | 0.36          |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 9        | 0.36          |
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 4        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2637) | 1:109:B:LEU:HA   | 1:122:B:GLY:HA2  | 8        | 0.36          |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG21 | 6        | 0.36          |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG22 | 6        | 0.36          |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG23 | 6        | 0.36          |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 1        | 0.36          |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 1        | 0.36          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 1        | 0.36          |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 8        | 0.36          |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 8        | 0.36          |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 8        | 0.36          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 10       | 0.36          |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 10       | 0.36          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 10       | 0.36          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 8        | 0.36          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 3        | 0.36          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 3        | 0.36          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 3        | 0.36          |
| (1,2314) | 1:94:B:ARG:HA    | 1:169:B:MET:HB2  | 8        | 0.36          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 5        | 0.36          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 5        | 0.36          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 5        | 0.36          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 5        | 0.36          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 5        | 0.36          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 5        | 0.36          |
| (1,1974) | 1:167:A:ALA:H    | 1:95:A:TRP:HB3   | 5        | 0.36          |
| (1,1916) | 1:162:A:THR:H    | 1:102:A:ASN:HB3  | 3        | 0.36          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 1        | 0.36          |
| (1,1642) | 1:132:A:GLY:H    | 1:129:A:ASP:HB2  | 3        | 0.36          |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD11 | 8        | 0.36          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 10       | 0.36          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 10       | 0.36          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 10       | 0.36          |
| (1,1332) | 1:95:A:TRP:H     | 1:95:A:TRP:HE3   | 4        | 0.36          |
| (1,1321) | 1:94:A:ARG:H     | 1:93:A:ASP:HA    | 8        | 0.36          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG21  | 10       | 0.36          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG22  | 10       | 0.36          |
| (1,1319) | 1:94:A:ARG:H     | 1:91:A:THR:HG23  | 10       | 0.36          |
| (1,1280) | 1:168:A:PRO:HB2  | 1:170:A:PRO:HD3  | 8        | 0.36          |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 3        | 0.36          |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 3        | 0.36          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 3        | 0.36          |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 5        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 7        | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 7        | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 7        | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 9        | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 9        | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 9        | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 10       | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 10       | 0.36          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 10       | 0.36          |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 9        | 0.36          |
| (1,990)  | 1:148:A:VAL:HA   | 1:169:A:MET:HB2  | 6        | 0.36          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 1        | 0.36          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 1        | 0.36          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 1        | 0.36          |
| (1,847)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HE3  | 7        | 0.36          |
| (1,826)  | 1:139:A:THR:HA   | 1:140:A:ARG:HB2  | 1        | 0.36          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD1  | 1        | 0.36          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD2  | 1        | 0.36          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD1  | 1        | 0.36          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD2  | 1        | 0.36          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD1  | 1        | 0.36          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD2  | 1        | 0.36          |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 4        | 0.36          |
| (1,695)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HB2  | 5        | 0.36          |
| (1,694)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HA   | 3        | 0.36          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 9        | 0.36          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 9        | 0.36          |
| (1,514)  | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 9        | 0.36          |
| (1,383)  | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 9        | 0.36          |
| (1,383)  | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 9        | 0.36          |
| (1,383)  | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 9        | 0.36          |
| (1,336)  | 1:108:A:GLU:HA   | 1:108:A:GLU:HG2  | 2        | 0.36          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 2        | 0.36          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 5        | 0.36          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 9        | 0.36          |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 1        | 0.36          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 2        | 0.36          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 2        | 0.36          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 2        | 0.36          |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 3        | 0.36          |
| (1,4290) | 1:171:B:LYS:H    | 1:171:B:LYS:HB3  | 4        | 0.35          |
| (1,4084) | 1:152:B:GLN:HE21 | 1:168:B:PRO:HD2  | 10       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 9        | 0.35          |
| (1,3915) | 1:131:B:HIS:H    | 1:129:B:ASP:HB3  | 2        | 0.35          |
| (1,3847) | 1:123:B:LYS:H    | 1:109:B:LEU:HB2  | 9        | 0.35          |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 7        | 0.35          |
| (1,3474) | 1:158:B:SER:HB3  | 1:160:B:GLU:HB3  | 3        | 0.35          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 6        | 0.35          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 5        | 0.35          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 4        | 0.35          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 4        | 0.35          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 4        | 0.35          |
| (1,3304) | 1:149:B:ASP:HA   | 1:149:B:ASP:HB3  | 5        | 0.35          |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 8        | 0.35          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 5        | 0.35          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 3        | 0.35          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 3        | 0.35          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 3        | 0.35          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 10       | 0.35          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 10       | 0.35          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 10       | 0.35          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 10       | 0.35          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 10       | 0.35          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 10       | 0.35          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 8        | 0.35          |
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 10       | 0.35          |
| (1,2971) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HB2  | 1        | 0.35          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 10       | 0.35          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 10       | 0.35          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 10       | 0.35          |
| (1,2755) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB3  | 4        | 0.35          |
| (1,2754) | 1:112:B:LYS:HE3  | 1:114:B:LYS:HB2  | 5        | 0.35          |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 9        | 0.35          |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 5        | 0.35          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 2        | 0.35          |
| (1,2629) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HE2  | 9        | 0.35          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 6        | 0.35          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 5        | 0.35          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 5        | 0.35          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 5        | 0.35          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 8        | 0.35          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 8        | 0.35          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 8        | 0.35          |
| (1,2536) | 1:99:B:LEU:HD21  | 1:109:B:LEU:HG   | 6        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2536) | 1:99:B:LEU:HD22  | 1:109:B:LEU:HG   | 6        | 0.35          |
| (1,2536) | 1:99:B:LEU:HD23  | 1:109:B:LEU:HG   | 6        | 0.35          |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB1  | 6        | 0.35          |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB2  | 6        | 0.35          |
| (1,2344) | 1:95:B:TRP:HB2   | 1:167:B:ALA:HB3  | 6        | 0.35          |
| (1,2299) | 1:93:B:ASP:HB2   | 1:94:B:ARG:HA    | 4        | 0.35          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 4        | 0.35          |
| (1,2286) | 1:90:B:HIS:HA    | 1:91:B:THR:HA    | 8        | 0.35          |
| (1,2213) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 8        | 0.35          |
| (1,2081) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 8        | 0.35          |
| (1,1816) | 1:153:A:VAL:H    | 1:149:A:ASP:HB2  | 9        | 0.35          |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 10       | 0.35          |
| (1,1423) | 1:108:A:GLU:H    | 1:123:A:LYS:HG2  | 3        | 0.35          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 4        | 0.35          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 5        | 0.35          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 5        | 0.35          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 5        | 0.35          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 5        | 0.35          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 9        | 0.35          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 9        | 0.35          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 9        | 0.35          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 9        | 0.35          |
| (1,1193) | 1:158:A:SER:HB3  | 1:160:A:GLU:HB3  | 8        | 0.35          |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 6        | 0.35          |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 6        | 0.35          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 6        | 0.35          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 8        | 0.35          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 10       | 0.35          |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 1        | 0.35          |
| (1,858)  | 1:141:A:LYS:HG3  | 1:141:A:LYS:HE2  | 10       | 0.35          |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE1  | 4        | 0.35          |
| (1,841)  | 1:140:A:ARG:HG2  | 1:142:A:TYR:HE2  | 4        | 0.35          |
| (1,826)  | 1:139:A:THR:HA   | 1:140:A:ARG:HB2  | 5        | 0.35          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 3        | 0.35          |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 1        | 0.35          |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 5        | 0.35          |
| (1,654)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD2  | 9        | 0.35          |
| (1,654)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD2  | 9        | 0.35          |
| (1,654)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD2  | 9        | 0.35          |
| (1,647)  | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 10       | 0.35          |
| (1,647)  | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 10       | 0.35          |
| (1,647)  | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 10       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,457)  | 1:112:A:LYS:HB2  | 1:120:A:ILE:HA   | 3        | 0.35          |
| (1,338)  | 1:108:A:GLU:HA   | 1:123:A:LYS:HD2  | 7        | 0.35          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 6        | 0.35          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 6        | 0.35          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 6        | 0.35          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 6        | 0.35          |
| (1,256)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 2        | 0.35          |
| (1,256)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 2        | 0.35          |
| (1,256)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 2        | 0.35          |
| (1,256)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 10       | 0.35          |
| (1,256)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 10       | 0.35          |
| (1,256)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 10       | 0.35          |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 3        | 0.35          |
| (1,71)   | 1:95:A:TRP:HB2   | 1:168:A:PRO:HB2  | 3        | 0.35          |
| (1,9)    | 1:90:A:HIS:HB3   | 1:91:A:THR:HA    | 2        | 0.35          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 9        | 0.35          |
| (1,4182) | 1:161:B:GLY:H    | 1:102:B:ASN:HB2  | 3        | 0.34          |
| (1,4051) | 1:151:B:THR:H    | 1:149:B:ASP:HB2  | 5        | 0.34          |
| (1,4024) | 1:148:B:VAL:H    | 1:146:B:PRO:HB3  | 4        | 0.34          |
| (1,3902) | 1:129:B:ASP:H    | 1:129:B:ASP:HB2  | 2        | 0.34          |
| (1,3833) | 1:121:B:THR:H    | 1:120:B:ILE:HG12 | 9        | 0.34          |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD21 | 9        | 0.34          |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD22 | 9        | 0.34          |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD23 | 9        | 0.34          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 1        | 0.34          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 1        | 0.34          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 1        | 0.34          |
| (1,3491) | 1:160:B:GLU:HB2  | 1:162:B:THR:HB   | 6        | 0.34          |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 5        | 0.34          |
| (1,3460) | 1:157:B:LEU:HD21 | 1:163:B:LEU:HB3  | 3        | 0.34          |
| (1,3460) | 1:157:B:LEU:HD22 | 1:163:B:LEU:HB3  | 3        | 0.34          |
| (1,3460) | 1:157:B:LEU:HD23 | 1:163:B:LEU:HB3  | 3        | 0.34          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 9        | 0.34          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 9        | 0.34          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 9        | 0.34          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 2        | 0.34          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD21 | 9        | 0.34          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD22 | 9        | 0.34          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD23 | 9        | 0.34          |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 6        | 0.34          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 6        | 0.34          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 7        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 7        | 0.34          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 7        | 0.34          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 7        | 0.34          |
| (1,3302) | 1:148:B:VAL:HG21 | 1:169:B:MET:HB3  | 1        | 0.34          |
| (1,3302) | 1:148:B:VAL:HG22 | 1:169:B:MET:HB3  | 1        | 0.34          |
| (1,3302) | 1:148:B:VAL:HG23 | 1:169:B:MET:HB3  | 1        | 0.34          |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 4        | 0.34          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 4        | 0.34          |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 10       | 0.34          |
| (1,2971) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HB2  | 4        | 0.34          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 10       | 0.34          |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 10       | 0.34          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 10       | 0.34          |
| (1,2686) | 1:110:B:THR:HG21 | 1:112:B:LYS:HD3  | 4        | 0.34          |
| (1,2686) | 1:110:B:THR:HG22 | 1:112:B:LYS:HD3  | 4        | 0.34          |
| (1,2686) | 1:110:B:THR:HG23 | 1:112:B:LYS:HD3  | 4        | 0.34          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 10       | 0.34          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 10       | 0.34          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 10       | 0.34          |
| (1,2629) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HE2  | 5        | 0.34          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD11 | 9        | 0.34          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD12 | 9        | 0.34          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD13 | 9        | 0.34          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 6        | 0.34          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 6        | 0.34          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 6        | 0.34          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB1  | 3        | 0.34          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB2  | 3        | 0.34          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB3  | 3        | 0.34          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 7        | 0.34          |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 8        | 0.34          |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 8        | 0.34          |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 8        | 0.34          |
| (1,2200) | 1:134:B:ILE:HG21 | 1:140:A:ARG:HD3  | 4        | 0.34          |
| (1,2200) | 1:134:B:ILE:HG22 | 1:140:A:ARG:HD3  | 4        | 0.34          |
| (1,2200) | 1:134:B:ILE:HG23 | 1:140:A:ARG:HD3  | 4        | 0.34          |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD3  | 10       | 0.34          |
| (1,2169) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 6        | 0.34          |
| (1,2169) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 7        | 0.34          |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 8        | 0.34          |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 8        | 0.34          |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 8        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2068) | 1:134:B:ILE:HG21 | 1:140:A:ARG:HD3  | 4        | 0.34          |
| (1,2068) | 1:134:B:ILE:HG22 | 1:140:A:ARG:HD3  | 4        | 0.34          |
| (1,2068) | 1:134:B:ILE:HG23 | 1:140:A:ARG:HD3  | 4        | 0.34          |
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD3  | 10       | 0.34          |
| (1,2037) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 6        | 0.34          |
| (1,2037) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 7        | 0.34          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 1        | 0.34          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 4        | 0.34          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD2   | 8        | 0.34          |
| (1,1805) | 1:152:A:GLN:HE21 | 1:170:A:PRO:HD3  | 7        | 0.34          |
| (1,1654) | 1:134:A:ILE:H    | 1:127:A:ARG:HB2  | 6        | 0.34          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD1  | 5        | 0.34          |
| (1,1630) | 1:129:A:ASP:H    | 1:133:A:TYR:HD2  | 5        | 0.34          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 7        | 0.34          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 10       | 0.34          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD11 | 3        | 0.34          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD12 | 3        | 0.34          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD13 | 3        | 0.34          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD21 | 8        | 0.34          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 4        | 0.34          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 4        | 0.34          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 4        | 0.34          |
| (1,1321) | 1:94:A:ARG:H     | 1:93:A:ASP:HA    | 5        | 0.34          |
| (1,1193) | 1:158:A:SER:HB3  | 1:160:A:GLU:HB3  | 6        | 0.34          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 4        | 0.34          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 1        | 0.34          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 1        | 0.34          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 1        | 0.34          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 8        | 0.34          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 2        | 0.34          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 4        | 0.34          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 5        | 0.34          |
| (1,1065) | 1:152:A:GLN:HB2  | 1:169:A:MET:HA   | 9        | 0.34          |
| (1,847)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HE3  | 1        | 0.34          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 2        | 0.34          |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 8        | 0.34          |
| (1,722)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HA   | 2        | 0.34          |
| (1,694)  | 1:123:A:LYS:HD2  | 1:137:A:CYS:HA   | 10       | 0.34          |
| (1,692)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 4        | 0.34          |
| (1,688)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB3  | 9        | 0.34          |
| (1,650)  | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD1  | 4        | 0.34          |
| (1,650)  | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD2  | 4        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,650)  | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD1  | 4        | 0.34          |
| (1,650)  | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD2  | 4        | 0.34          |
| (1,650)  | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD1  | 4        | 0.34          |
| (1,650)  | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD2  | 4        | 0.34          |
| (1,478)  | 1:112:A:LYS:HE3  | 1:121:A:THR:HB   | 9        | 0.34          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 4        | 0.34          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 8        | 0.34          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD11 | 5        | 0.34          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD12 | 5        | 0.34          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD13 | 5        | 0.34          |
| (1,256)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 9        | 0.34          |
| (1,256)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 9        | 0.34          |
| (1,256)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 9        | 0.34          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 4        | 0.34          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 4        | 0.34          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 4        | 0.34          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 2        | 0.34          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 2        | 0.34          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 2        | 0.34          |
| (1,102)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HB3  | 2        | 0.34          |
| (1,99)   | 1:96:A:ARG:HB3   | 1:164:A:THR:HB   | 9        | 0.34          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 1        | 0.34          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 1        | 0.34          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 1        | 0.34          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 1        | 0.34          |
| (1,69)   | 1:95:A:TRP:HB3   | 1:166:A:GLU:HB2  | 6        | 0.34          |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG21 | 9        | 0.33          |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG22 | 9        | 0.33          |
| (1,4221) | 1:164:B:THR:H    | 1:162:B:THR:HG23 | 9        | 0.33          |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 9        | 0.33          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 2        | 0.33          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 1        | 0.33          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 1        | 0.33          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 1        | 0.33          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 6        | 0.33          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 6        | 0.33          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 6        | 0.33          |
| (1,3935) | 1:134:B:ILE:H    | 1:127:B:ARG:HB2  | 2        | 0.33          |
| (1,3907) | 1:129:B:ASP:H    | 1:132:B:GLY:HA3  | 8        | 0.33          |
| (1,3847) | 1:123:B:LYS:H    | 1:109:B:LEU:HB2  | 2        | 0.33          |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD11 | 8        | 0.33          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 5        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 5        | 0.33          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 5        | 0.33          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 4        | 0.33          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 4        | 0.33          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 4        | 0.33          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 8        | 0.33          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 8        | 0.33          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 8        | 0.33          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 3        | 0.33          |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 5        | 0.33          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 6        | 0.33          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 1        | 0.33          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 1        | 0.33          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 1        | 0.33          |
| (1,3120) | 1:140:B:ARG:HB2  | 1:140:B:ARG:HD2  | 4        | 0.33          |
| (1,3060) | 1:131:B:HIS:HA   | 1:131:B:HIS:HE1  | 3        | 0.33          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 7        | 0.33          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 7        | 0.33          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 7        | 0.33          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 8        | 0.33          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 8        | 0.33          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 8        | 0.33          |
| (1,2753) | 1:112:B:LYS:HD3  | 1:120:B:ILE:HA   | 8        | 0.33          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE3  | 1        | 0.33          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 3        | 0.33          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 3        | 0.33          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 3        | 0.33          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 8        | 0.33          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 8        | 0.33          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 8        | 0.33          |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 2        | 0.33          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 2        | 0.33          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 2        | 0.33          |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 10       | 0.33          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 10       | 0.33          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 10       | 0.33          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD11 | 10       | 0.33          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD12 | 10       | 0.33          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD13 | 10       | 0.33          |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 10       | 0.33          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 9        | 0.33          |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD3  | 2        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD21 | 7        | 0.33          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD22 | 7        | 0.33          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD23 | 7        | 0.33          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 7        | 0.33          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 10       | 0.33          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 10       | 0.33          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 10       | 0.33          |
| (1,2568) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB3  | 3        | 0.33          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 1        | 0.33          |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 9        | 0.33          |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 9        | 0.33          |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 9        | 0.33          |
| (1,2299) | 1:93:B:ASP:HB2   | 1:94:B:ARG:HA    | 1        | 0.33          |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 8        | 0.33          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 7        | 0.33          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 7        | 0.33          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 7        | 0.33          |
| (1,2150) | 1:97:B:VAL:HG21  | 1:131:A:HIS:HB3  | 9        | 0.33          |
| (1,2150) | 1:97:B:VAL:HG22  | 1:131:A:HIS:HB3  | 9        | 0.33          |
| (1,2150) | 1:97:B:VAL:HG23  | 1:131:A:HIS:HB3  | 9        | 0.33          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 7        | 0.33          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 7        | 0.33          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 7        | 0.33          |
| (1,2018) | 1:97:B:VAL:HG21  | 1:131:A:HIS:HB3  | 9        | 0.33          |
| (1,2018) | 1:97:B:VAL:HG22  | 1:131:A:HIS:HB3  | 9        | 0.33          |
| (1,2018) | 1:97:B:VAL:HG23  | 1:131:A:HIS:HB3  | 9        | 0.33          |
| (1,1847) | 1:155:A:SER:H    | 1:154:A:SER:HB2  | 9        | 0.33          |
| (1,1634) | 1:131:A:HIS:H    | 1:129:A:ASP:HB3  | 3        | 0.33          |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 6        | 0.33          |
| (1,1587) | 1:126:A:GLU:H    | 1:125:A:GLU:HG2  | 2        | 0.33          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 4        | 0.33          |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 1        | 0.33          |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 6        | 0.33          |
| (1,1179) | 1:157:A:LEU:HD21 | 1:163:A:LEU:HB3  | 8        | 0.33          |
| (1,1179) | 1:157:A:LEU:HD22 | 1:163:A:LEU:HB3  | 8        | 0.33          |
| (1,1179) | 1:157:A:LEU:HD23 | 1:163:A:LEU:HB3  | 8        | 0.33          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 3        | 0.33          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD21 | 4        | 0.33          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD22 | 4        | 0.33          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD23 | 4        | 0.33          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 3        | 0.33          |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 2        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 9        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD1  | 3        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD2  | 3        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD1  | 3        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD2  | 3        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD1  | 3        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD2  | 3        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD1  | 4        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD2  | 4        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD1  | 4        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD2  | 4        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD1  | 4        | 0.33          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD2  | 4        | 0.33          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE1  | 7        | 0.33          |
| (1,754)  | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE2  | 7        | 0.33          |
| (1,707)  | 1:126:A:GLU:HA   | 1:133:A:TYR:HB3  | 2        | 0.33          |
| (1,703)  | 1:125:A:GLU:HA   | 1:135:A:SER:HB2  | 4        | 0.33          |
| (1,695)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HB2  | 7        | 0.33          |
| (1,612)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HE3  | 7        | 0.33          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 4        | 0.33          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 4        | 0.33          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 4        | 0.33          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 4        | 0.33          |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 4        | 0.33          |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 4        | 0.33          |
| (1,528)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HB   | 7        | 0.33          |
| (1,453)  | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 4        | 0.33          |
| (1,434)  | 1:111:A:VAL:HG11 | 1:120:A:ILE:HG12 | 6        | 0.33          |
| (1,434)  | 1:111:A:VAL:HG12 | 1:120:A:ILE:HG12 | 6        | 0.33          |
| (1,434)  | 1:111:A:VAL:HG13 | 1:120:A:ILE:HG12 | 6        | 0.33          |
| (1,406)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HE3  | 3        | 0.33          |
| (1,406)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HE3  | 3        | 0.33          |
| (1,406)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HE3  | 3        | 0.33          |
| (1,373)  | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 9        | 0.33          |
| (1,373)  | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 9        | 0.33          |
| (1,373)  | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 9        | 0.33          |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 4        | 0.33          |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 4        | 0.33          |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 4        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 9        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 9        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 9        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 9        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 9        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 9        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 9        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 9        | 0.33          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 9        | 0.33          |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 1        | 0.33          |
| (1,166)  | 1:97:A:VAL:HG21  | 1:118:A:VAL:HB   | 9        | 0.33          |
| (1,166)  | 1:97:A:VAL:HG22  | 1:118:A:VAL:HB   | 9        | 0.33          |
| (1,166)  | 1:97:A:VAL:HG23  | 1:118:A:VAL:HB   | 9        | 0.33          |
| (1,102)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HB3  | 9        | 0.33          |
| (1,99)   | 1:96:A:ARG:HB3   | 1:164:A:THR:HB   | 2        | 0.33          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 9        | 0.33          |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 4        | 0.33          |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 2        | 0.33          |
| (1,4290) | 1:171:B:LYS:H    | 1:171:B:LYS:HB2  | 5        | 0.32          |
| (1,4281) | 1:169:B:MET:H    | 1:169:B:MET:HG3  | 9        | 0.32          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB1   | 10       | 0.32          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB2   | 10       | 0.32          |
| (1,4268) | 1:169:B:MET:H    | 1:92:B:ALA:HB3   | 10       | 0.32          |
| (1,4255) | 1:167:B:ALA:H    | 1:95:B:TRP:HB3   | 1        | 0.32          |
| (1,4205) | 1:162:B:THR:H    | 1:160:B:GLU:HB2  | 9        | 0.32          |
| (1,4197) | 1:162:B:THR:H    | 1:102:B:ASN:HB3  | 6        | 0.32          |
| (1,4128) | 1:155:B:SER:H    | 1:154:B:SER:HB2  | 7        | 0.32          |
| (1,3955) | 1:137:B:CYS:H    | 1:136:B:ARG:HB3  | 9        | 0.32          |
| (1,3847) | 1:123:B:LYS:H    | 1:109:B:LEU:HB2  | 3        | 0.32          |
| (1,3847) | 1:123:B:LYS:H    | 1:109:B:LEU:HB2  | 5        | 0.32          |
| (1,3827) | 1:120:B:ILE:H    | 1:142:B:TYR:H    | 2        | 0.32          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 4        | 0.32          |
| (1,3825) | 1:120:B:ILE:H    | 1:140:B:ARG:HG2  | 2        | 0.32          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 1        | 0.32          |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD21 | 1        | 0.32          |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD22 | 1        | 0.32          |
| (1,3653) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD23 | 1        | 0.32          |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD21 | 4        | 0.32          |
| (1,3613) | 1:95:B:TRP:H     | 1:95:B:TRP:HE3   | 8        | 0.32          |
| (1,3604) | 1:94:B:ARG:H     | 1:93:B:ASP:HB3   | 1        | 0.32          |
| (1,3602) | 1:94:B:ARG:H     | 1:93:B:ASP:HA    | 4        | 0.32          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 6        | 0.32          |
| (1,3561) | 1:168:B:PRO:HB2  | 1:170:B:PRO:HD3  | 9        | 0.32          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 1        | 0.32          |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 4        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 7        | 0.32          |
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 7        | 0.32          |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 7        | 0.32          |
| (1,3096) | 1:136:B:ARG:HG3  | 1:138:B:PHE:HA   | 9        | 0.32          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 10       | 0.32          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 10       | 0.32          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 1        | 0.32          |
| (1,2929) | 1:120:B:ILE:HG21 | 1:139:B:THR:HA   | 10       | 0.32          |
| (1,2929) | 1:120:B:ILE:HG22 | 1:139:B:THR:HA   | 10       | 0.32          |
| (1,2929) | 1:120:B:ILE:HG23 | 1:139:B:THR:HA   | 10       | 0.32          |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 7        | 0.32          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 2        | 0.32          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 2        | 0.32          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 2        | 0.32          |
| (1,2617) | 1:108:B:GLU:HA   | 1:108:B:GLU:HG2  | 5        | 0.32          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 4        | 0.32          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 7        | 0.32          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 3        | 0.32          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 3        | 0.32          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 3        | 0.32          |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 6        | 0.32          |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 6        | 0.32          |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 6        | 0.32          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 1        | 0.32          |
| (1,2282) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HA    | 1        | 0.32          |
| (1,2282) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HA    | 1        | 0.32          |
| (1,2282) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HA    | 1        | 0.32          |
| (1,1974) | 1:167:A:ALA:H    | 1:95:A:TRP:HB3   | 7        | 0.32          |
| (1,1894) | 1:160:A:GLU:H    | 1:159:A:PRO:HG2  | 2        | 0.32          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG21 | 2        | 0.32          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG22 | 2        | 0.32          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG23 | 2        | 0.32          |
| (1,1814) | 1:152:A:GLN:HE22 | 1:170:A:PRO:HD3  | 2        | 0.32          |
| (1,1794) | 1:152:A:GLN:H    | 1:168:A:PRO:HD3  | 1        | 0.32          |
| (1,1756) | 1:148:A:VAL:H    | 1:170:A:PRO:HG3  | 9        | 0.32          |
| (1,1664) | 1:135:A:SER:H    | 1:134:A:ILE:HG13 | 1        | 0.32          |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 3        | 0.32          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 3        | 0.32          |
| (1,1322) | 1:94:A:ARG:H     | 1:93:A:ASP:HB2   | 7        | 0.32          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 9        | 0.32          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 9        | 0.32          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 9        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 10       | 0.32          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 10       | 0.32          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 10       | 0.32          |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 3        | 0.32          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 7        | 0.32          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 6        | 0.32          |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG3  | 6        | 0.32          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 8        | 0.32          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 8        | 0.32          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 8        | 0.32          |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 4        | 0.32          |
| (1,835)  | 1:139:A:THR:HG21 | 1:141:A:LYS:HE2  | 9        | 0.32          |
| (1,835)  | 1:139:A:THR:HG22 | 1:141:A:LYS:HE2  | 9        | 0.32          |
| (1,835)  | 1:139:A:THR:HG23 | 1:141:A:LYS:HE2  | 9        | 0.32          |
| (1,715)  | 1:126:A:GLU:HB2  | 1:135:A:SER:HB3  | 7        | 0.32          |
| (1,693)  | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB3  | 10       | 0.32          |
| (1,650)  | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD1  | 9        | 0.32          |
| (1,650)  | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD2  | 9        | 0.32          |
| (1,650)  | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD1  | 9        | 0.32          |
| (1,650)  | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD2  | 9        | 0.32          |
| (1,650)  | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD1  | 9        | 0.32          |
| (1,650)  | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD2  | 9        | 0.32          |
| (1,639)  | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 3        | 0.32          |
| (1,635)  | 1:120:A:ILE:HB   | 1:140:A:ARG:HD2  | 10       | 0.32          |
| (1,509)  | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 1        | 0.32          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 1        | 0.32          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 6        | 0.32          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 5        | 0.32          |
| (1,42)   | 1:94:A:ARG:HB3   | 1:168:A:PRO:HA   | 1        | 0.32          |
| (1,7)    | 1:90:A:HIS:HB2   | 1:91:A:THR:HA    | 6        | 0.32          |
| (1,4205) | 1:162:B:THR:H    | 1:160:B:GLU:HB2  | 10       | 0.31          |
| (1,4128) | 1:155:B:SER:H    | 1:154:B:SER:HB2  | 4        | 0.31          |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 4        | 0.31          |
| (1,4065) | 1:152:B:GLN:H    | 1:149:B:ASP:HB3  | 3        | 0.31          |
| (1,3935) | 1:134:B:ILE:H    | 1:127:B:ARG:HB2  | 3        | 0.31          |
| (1,3862) | 1:125:B:GLU:H    | 1:108:B:GLU:HG3  | 4        | 0.31          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 1        | 0.31          |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 5        | 0.31          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 10       | 0.31          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 10       | 0.31          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 10       | 0.31          |
| (1,3492) | 1:160:B:GLU:HG2  | 1:162:B:THR:HB   | 1        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 1        | 0.31          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 7        | 0.31          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 4        | 0.31          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 8        | 0.31          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 5        | 0.31          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 10       | 0.31          |
| (1,3209) | 1:144:B:LEU:HD11 | 1:145:B:PRO:HB3  | 3        | 0.31          |
| (1,3209) | 1:144:B:LEU:HD12 | 1:145:B:PRO:HB3  | 3        | 0.31          |
| (1,3209) | 1:144:B:LEU:HD13 | 1:145:B:PRO:HB3  | 3        | 0.31          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 4        | 0.31          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 4        | 0.31          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 4        | 0.31          |
| (1,3139) | 1:141:B:LYS:HG3  | 1:141:B:LYS:HE2  | 1        | 0.31          |
| (1,3139) | 1:141:B:LYS:HG3  | 1:141:B:LYS:HE2  | 2        | 0.31          |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 1        | 0.31          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 5        | 0.31          |
| (1,3018) | 1:127:B:ARG:HA   | 1:127:B:ARG:HD3  | 1        | 0.31          |
| (1,3018) | 1:127:B:ARG:HA   | 1:127:B:ARG:HD3  | 2        | 0.31          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE1  | 10       | 0.31          |
| (1,3012) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HE2  | 10       | 0.31          |
| (1,2975) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HA   | 3        | 0.31          |
| (1,2975) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HA   | 4        | 0.31          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG21 | 4        | 0.31          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG22 | 4        | 0.31          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG23 | 4        | 0.31          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG21 | 8        | 0.31          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG22 | 8        | 0.31          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG23 | 8        | 0.31          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 10       | 0.31          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 10       | 0.31          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 10       | 0.31          |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 5        | 0.31          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 5        | 0.31          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 5        | 0.31          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD11 | 1        | 0.31          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD12 | 1        | 0.31          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD13 | 1        | 0.31          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 9        | 0.31          |
| (1,2601) | 1:106:B:PRO:HB2  | 1:106:B:PRO:HD3  | 3        | 0.31          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 1        | 0.31          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 1        | 0.31          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 1        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 3        | 0.31          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 3        | 0.31          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 3        | 0.31          |
| (1,2377) | 1:96:B:ARG:HB2   | 1:166:B:GLU:HB2  | 5        | 0.31          |
| (1,2353) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB3  | 9        | 0.31          |
| (1,2352) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB2  | 5        | 0.31          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 6        | 0.31          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 6        | 0.31          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 6        | 0.31          |
| (1,2330) | 1:94:B:ARG:HD3   | 1:168:B:PRO:HA   | 8        | 0.31          |
| (1,2329) | 1:94:B:ARG:HD2   | 1:168:B:PRO:HA   | 7        | 0.31          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 1        | 0.31          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 1        | 0.31          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 1        | 0.31          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 1        | 0.31          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 1        | 0.31          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 1        | 0.31          |
| (1,1998) | 1:169:A:MET:H    | 1:169:A:MET:HB2  | 5        | 0.31          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD2   | 4        | 0.31          |
| (1,1902) | 1:161:A:GLY:H    | 1:102:A:ASN:HB3  | 2        | 0.31          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 9        | 0.31          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 9        | 0.31          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 9        | 0.31          |
| (1,1640) | 1:132:A:GLY:H    | 1:128:A:GLN:HG2  | 1        | 0.31          |
| (1,1634) | 1:131:A:HIS:H    | 1:129:A:ASP:HB3  | 7        | 0.31          |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 3        | 0.31          |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 8        | 0.31          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 1        | 0.31          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 1        | 0.31          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 1        | 0.31          |
| (1,1323) | 1:94:A:ARG:H     | 1:93:A:ASP:HB3   | 4        | 0.31          |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 6        | 0.31          |
| (1,1163) | 1:157:A:LEU:HG   | 1:161:A:GLY:HA3  | 8        | 0.31          |
| (1,1085) | 1:153:A:VAL:HG11 | 1:155:A:SER:HB3  | 6        | 0.31          |
| (1,1085) | 1:153:A:VAL:HG12 | 1:155:A:SER:HB3  | 6        | 0.31          |
| (1,1085) | 1:153:A:VAL:HG13 | 1:155:A:SER:HB3  | 6        | 0.31          |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 5        | 0.31          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 2        | 0.31          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 2        | 0.31          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 2        | 0.31          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG11 | 10       | 0.31          |
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG12 | 10       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,974)  | 1:147:A:GLY:HA2  | 1:148:A:VAL:HG13 | 10       | 0.31          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG11 | 6        | 0.31          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG12 | 6        | 0.31          |
| (1,959)  | 1:145:A:PRO:HG3  | 1:148:A:VAL:HG13 | 6        | 0.31          |
| (1,930)  | 1:144:A:LEU:HD11 | 1:148:A:VAL:HA   | 10       | 0.31          |
| (1,930)  | 1:144:A:LEU:HD12 | 1:148:A:VAL:HA   | 10       | 0.31          |
| (1,930)  | 1:144:A:LEU:HD13 | 1:148:A:VAL:HA   | 10       | 0.31          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 10       | 0.31          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 10       | 0.31          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 10       | 0.31          |
| (1,827)  | 1:139:A:THR:HA   | 1:140:A:ARG:HG2  | 9        | 0.31          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 4        | 0.31          |
| (1,746)  | 1:128:A:GLN:HA   | 1:128:A:GLN:HG3  | 2        | 0.31          |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 2        | 0.31          |
| (1,694)  | 1:123:A:LYS:HD2  | 1:137:A:CYS:HA   | 1        | 0.31          |
| (1,648)  | 1:120:A:ILE:HG21 | 1:139:A:THR:HA   | 1        | 0.31          |
| (1,648)  | 1:120:A:ILE:HG22 | 1:139:A:THR:HA   | 1        | 0.31          |
| (1,648)  | 1:120:A:ILE:HG23 | 1:139:A:THR:HA   | 1        | 0.31          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG21 | 1        | 0.31          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG22 | 1        | 0.31          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG23 | 1        | 0.31          |
| (1,528)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HB   | 2        | 0.31          |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 10       | 0.31          |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 10       | 0.31          |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 10       | 0.31          |
| (1,418)  | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 4        | 0.31          |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD3  | 6        | 0.31          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 3        | 0.31          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 5        | 0.31          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 3        | 0.31          |
| (1,320)  | 1:106:A:PRO:HB2  | 1:106:A:PRO:HD3  | 10       | 0.31          |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 5        | 0.31          |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 5        | 0.31          |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 5        | 0.31          |
| (1,280)  | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA3  | 3        | 0.31          |
| (1,155)  | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 7        | 0.31          |
| (1,155)  | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 7        | 0.31          |
| (1,155)  | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 7        | 0.31          |
| (1,4280) | 1:169:B:MET:H    | 1:169:B:MET:HB3  | 8        | 0.3           |
| (1,4205) | 1:162:B:THR:H    | 1:160:B:GLU:HB2  | 2        | 0.3           |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 1        | 0.3           |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 1        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 1        | 0.3           |
| (1,3915) | 1:131:B:HIS:H    | 1:129:B:ASP:HB3  | 7        | 0.3           |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 8        | 0.3           |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 2        | 0.3           |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 2        | 0.3           |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 2        | 0.3           |
| (1,3491) | 1:160:B:GLU:HB2  | 1:162:B:THR:HB   | 7        | 0.3           |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 3        | 0.3           |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 9        | 0.3           |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD11 | 9        | 0.3           |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD12 | 9        | 0.3           |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD13 | 9        | 0.3           |
| (1,3400) | 1:155:B:SER:HB2  | 1:165:B:VAL:HA   | 5        | 0.3           |
| (1,3378) | 1:154:B:SER:HB3  | 1:155:B:SER:HA   | 7        | 0.3           |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 7        | 0.3           |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 2        | 0.3           |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 10       | 0.3           |
| (1,3018) | 1:127:B:ARG:HA   | 1:127:B:ARG:HD3  | 7        | 0.3           |
| (1,2996) | 1:126:B:GLU:HB2  | 1:135:B:SER:HB3  | 7        | 0.3           |
| (1,2977) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB3  | 10       | 0.3           |
| (1,2975) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HA   | 1        | 0.3           |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG21 | 1        | 0.3           |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG22 | 1        | 0.3           |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG23 | 1        | 0.3           |
| (1,2891) | 1:119:B:GLU:HA   | 1:141:B:LYS:HD3  | 6        | 0.3           |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 7        | 0.3           |
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 7        | 0.3           |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 7        | 0.3           |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE3  | 8        | 0.3           |
| (1,2715) | 1:111:B:VAL:HG11 | 1:120:B:ILE:HG12 | 5        | 0.3           |
| (1,2715) | 1:111:B:VAL:HG12 | 1:120:B:ILE:HG12 | 5        | 0.3           |
| (1,2715) | 1:111:B:VAL:HG13 | 1:120:B:ILE:HG12 | 5        | 0.3           |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD11 | 7        | 0.3           |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD12 | 7        | 0.3           |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD13 | 7        | 0.3           |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 5        | 0.3           |
| (1,2626) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HE3  | 6        | 0.3           |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 3        | 0.3           |
| (1,2539) | 1:99:B:LEU:HD21  | 1:120:B:ILE:HA   | 10       | 0.3           |
| (1,2539) | 1:99:B:LEU:HD22  | 1:120:B:ILE:HA   | 10       | 0.3           |
| (1,2539) | 1:99:B:LEU:HD23  | 1:120:B:ILE:HA   | 10       | 0.3           |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 4        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 4        | 0.3           |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 4        | 0.3           |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE1  | 6        | 0.3           |
| (1,2535) | 1:99:B:LEU:HD21  | 1:142:B:TYR:HE2  | 6        | 0.3           |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE1  | 6        | 0.3           |
| (1,2535) | 1:99:B:LEU:HD22  | 1:142:B:TYR:HE2  | 6        | 0.3           |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE1  | 6        | 0.3           |
| (1,2535) | 1:99:B:LEU:HD23  | 1:142:B:TYR:HE2  | 6        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG21 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG22 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG23 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG21 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG22 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG23 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG21 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG22 | 3        | 0.3           |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG23 | 3        | 0.3           |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 5        | 0.3           |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 5        | 0.3           |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 5        | 0.3           |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 9        | 0.3           |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 9        | 0.3           |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 9        | 0.3           |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 7        | 0.3           |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 7        | 0.3           |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 7        | 0.3           |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 8        | 0.3           |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 8        | 0.3           |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 8        | 0.3           |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG21 | 5        | 0.3           |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG22 | 5        | 0.3           |
| (1,2349) | 1:95:B:TRP:HB3   | 1:148:B:VAL:HG23 | 5        | 0.3           |
| (1,2312) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD2  | 2        | 0.3           |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB1   | 2        | 0.3           |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB2   | 2        | 0.3           |
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB3   | 2        | 0.3           |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 6        | 0.3           |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 6        | 0.3           |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 6        | 0.3           |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 6        | 0.3           |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 6        | 0.3           |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 6        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1915) | 1:162:A:THR:H    | 1:102:A:ASN:HB2  | 10       | 0.3           |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 2        | 0.3           |
| (1,1847) | 1:155:A:SER:H    | 1:154:A:SER:HB2  | 7        | 0.3           |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 8        | 0.3           |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 8        | 0.3           |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 8        | 0.3           |
| (1,1654) | 1:134:A:ILE:H    | 1:127:A:ARG:HB2  | 2        | 0.3           |
| (1,1598) | 1:128:A:GLN:H    | 1:127:A:ARG:HG2  | 7        | 0.3           |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 9        | 0.3           |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 6        | 0.3           |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 8        | 0.3           |
| (1,1411) | 1:108:A:GLU:H    | 1:105:A:ALA:HA   | 6        | 0.3           |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 2        | 0.3           |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 3        | 0.3           |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 2        | 0.3           |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 2        | 0.3           |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 2        | 0.3           |
| (1,1219) | 1:162:A:THR:HA   | 1:162:A:THR:HG21 | 2        | 0.3           |
| (1,1219) | 1:162:A:THR:HA   | 1:162:A:THR:HG22 | 2        | 0.3           |
| (1,1219) | 1:162:A:THR:HA   | 1:162:A:THR:HG23 | 2        | 0.3           |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 10       | 0.3           |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 1        | 0.3           |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 4        | 0.3           |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 4        | 0.3           |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 4        | 0.3           |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 3        | 0.3           |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 3        | 0.3           |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 3        | 0.3           |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 1        | 0.3           |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 10       | 0.3           |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 8        | 0.3           |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 8        | 0.3           |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 8        | 0.3           |
| (1,1012) | 1:148:A:VAL:HG11 | 1:169:A:MET:HB2  | 2        | 0.3           |
| (1,1012) | 1:148:A:VAL:HG12 | 1:169:A:MET:HB2  | 2        | 0.3           |
| (1,1012) | 1:148:A:VAL:HG13 | 1:169:A:MET:HB2  | 2        | 0.3           |
| (1,920)  | 1:144:A:LEU:HB3  | 1:148:A:VAL:HG21 | 6        | 0.3           |
| (1,920)  | 1:144:A:LEU:HB3  | 1:148:A:VAL:HG22 | 6        | 0.3           |
| (1,920)  | 1:144:A:LEU:HB3  | 1:148:A:VAL:HG23 | 6        | 0.3           |
| (1,777)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HB3  | 2        | 0.3           |
| (1,723)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB2  | 10       | 0.3           |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 9        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,690)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HB2  | 6        | 0.3           |
| (1,684)  | 1:123:A:LYS:HA   | 1:135:A:SER:HB3  | 4        | 0.3           |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 8        | 0.3           |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 8        | 0.3           |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 8        | 0.3           |
| (1,639)  | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 8        | 0.3           |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 1        | 0.3           |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 1        | 0.3           |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 1        | 0.3           |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 7        | 0.3           |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 7        | 0.3           |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 7        | 0.3           |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 2        | 0.3           |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 2        | 0.3           |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 2        | 0.3           |
| (1,383)  | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 2        | 0.3           |
| (1,383)  | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 2        | 0.3           |
| (1,383)  | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 2        | 0.3           |
| (1,359)  | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 9        | 0.3           |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 7        | 0.3           |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 10       | 0.3           |
| (1,258)  | 1:99:A:LEU:HD21  | 1:120:A:ILE:HA   | 1        | 0.3           |
| (1,258)  | 1:99:A:LEU:HD22  | 1:120:A:ILE:HA   | 1        | 0.3           |
| (1,258)  | 1:99:A:LEU:HD23  | 1:120:A:ILE:HA   | 1        | 0.3           |
| (1,186)  | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 4        | 0.3           |
| (1,80)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HD2   | 7        | 0.3           |
| (1,19)   | 1:93:A:ASP:HB2   | 1:94:A:ARG:HG2   | 2        | 0.3           |
| (1,5)    | 1:90:A:HIS:HA    | 1:91:A:THR:HA    | 6        | 0.3           |
| (1,3972) | 1:140:B:ARG:H    | 1:120:B:ILE:HB   | 6        | 0.29          |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG2  | 4        | 0.29          |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 1        | 0.29          |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 2        | 0.29          |
| (1,3748) | 1:113:B:THR:H    | 1:112:B:LYS:HB2  | 2        | 0.29          |
| (1,3726) | 1:111:B:VAL:H    | 1:110:B:THR:HB   | 7        | 0.29          |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 7        | 0.29          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 5        | 0.29          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 7        | 0.29          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 7        | 0.29          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 7        | 0.29          |
| (1,3599) | 1:171:B:LYS:HA   | 1:171:B:LYS:HD3  | 1        | 0.29          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 5        | 0.29          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 1        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 7        | 0.29          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 2        | 0.29          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 2        | 0.29          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 2        | 0.29          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG21 | 4        | 0.29          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG22 | 4        | 0.29          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG23 | 4        | 0.29          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 5        | 0.29          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 5        | 0.29          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 5        | 0.29          |
| (1,3139) | 1:141:B:LYS:HG3  | 1:141:B:LYS:HE2  | 8        | 0.29          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD1  | 7        | 0.29          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD2  | 7        | 0.29          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD1  | 7        | 0.29          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD2  | 7        | 0.29          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD1  | 7        | 0.29          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD2  | 7        | 0.29          |
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 7        | 0.29          |
| (1,2977) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB3  | 1        | 0.29          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 10       | 0.29          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 10       | 0.29          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 10       | 0.29          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG21 | 10       | 0.29          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG22 | 10       | 0.29          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG23 | 10       | 0.29          |
| (1,2715) | 1:111:B:VAL:HG11 | 1:120:B:ILE:HG12 | 2        | 0.29          |
| (1,2715) | 1:111:B:VAL:HG12 | 1:120:B:ILE:HG12 | 2        | 0.29          |
| (1,2715) | 1:111:B:VAL:HG13 | 1:120:B:ILE:HG12 | 2        | 0.29          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 4        | 0.29          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 4        | 0.29          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 4        | 0.29          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD11 | 8        | 0.29          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD12 | 8        | 0.29          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD13 | 8        | 0.29          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 1        | 0.29          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 8        | 0.29          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 10       | 0.29          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 10       | 0.29          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 10       | 0.29          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 7        | 0.29          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 7        | 0.29          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 7        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG11 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG12 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG13 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG11 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG12 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG13 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG11 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG12 | 6        | 0.29          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG13 | 6        | 0.29          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 2        | 0.29          |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 2        | 0.29          |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 4        | 0.29          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB1  | 10       | 0.29          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB2  | 10       | 0.29          |
| (1,2358) | 1:95:B:TRP:HE3   | 1:167:B:ALA:HB3  | 10       | 0.29          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 1        | 0.29          |
| (1,2285) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB3   | 5        | 0.29          |
| (1,2284) | 1:89:B:ARG:HB3   | 1:90:B:HIS:HB2   | 9        | 0.29          |
| (1,1998) | 1:169:A:MET:H    | 1:169:A:MET:HB2  | 8        | 0.29          |
| (1,1847) | 1:155:A:SER:H    | 1:154:A:SER:HB2  | 4        | 0.29          |
| (1,1650) | 1:132:A:GLY:H    | 1:133:A:TYR:HD1  | 1        | 0.29          |
| (1,1650) | 1:132:A:GLY:H    | 1:133:A:TYR:HD2  | 1        | 0.29          |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 1        | 0.29          |
| (1,1500) | 1:117:A:VAL:H    | 1:115:A:ASP:HB2  | 10       | 0.29          |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 7        | 0.29          |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD11 | 2        | 0.29          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD11 | 10       | 0.29          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD12 | 10       | 0.29          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD13 | 10       | 0.29          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD21 | 1        | 0.29          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD22 | 1        | 0.29          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD23 | 1        | 0.29          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG21 | 6        | 0.29          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG22 | 6        | 0.29          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG23 | 6        | 0.29          |
| (1,1318) | 1:171:A:LYS:HA   | 1:171:A:LYS:HD3  | 8        | 0.29          |
| (1,1276) | 1:168:A:PRO:HA   | 1:169:A:MET:HG2  | 9        | 0.29          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 8        | 0.29          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 8        | 0.29          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 8        | 0.29          |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 1        | 0.29          |
| (1,1197) | 1:158:A:SER:HB3  | 1:159:A:PRO:HD3  | 9        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 5        | 0.29          |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 1        | 0.29          |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 6        | 0.29          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 9        | 0.29          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 3        | 0.29          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 3        | 0.29          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 3        | 0.29          |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 3        | 0.29          |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 7        | 0.29          |
| (1,1065) | 1:152:A:GLN:HB2  | 1:169:A:MET:HA   | 7        | 0.29          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 2        | 0.29          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 6        | 0.29          |
| (1,1012) | 1:148:A:VAL:HG11 | 1:169:A:MET:HB2  | 6        | 0.29          |
| (1,1012) | 1:148:A:VAL:HG12 | 1:169:A:MET:HB2  | 6        | 0.29          |
| (1,1012) | 1:148:A:VAL:HG13 | 1:169:A:MET:HB2  | 6        | 0.29          |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 6        | 0.29          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 6        | 0.29          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 6        | 0.29          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 6        | 0.29          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG11 | 8        | 0.29          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG12 | 8        | 0.29          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG13 | 8        | 0.29          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG11 | 8        | 0.29          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG12 | 8        | 0.29          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG13 | 8        | 0.29          |
| (1,847)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HE3  | 6        | 0.29          |
| (1,808)  | 1:135:A:SER:HA   | 1:135:A:SER:HB2  | 5        | 0.29          |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG22 | 1        | 0.29          |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 7        | 0.29          |
| (1,688)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB3  | 2        | 0.29          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 10       | 0.29          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 10       | 0.29          |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 8        | 0.29          |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 8        | 0.29          |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 8        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,404)  | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 6        | 0.29          |
| (1,404)  | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 6        | 0.29          |
| (1,404)  | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 6        | 0.29          |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD2  | 7        | 0.29          |
| (1,324)  | 1:106:A:PRO:HB3  | 1:107:A:ASP:HA   | 9        | 0.29          |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 3        | 0.29          |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 3        | 0.29          |
| (1,289)  | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 3        | 0.29          |
| (1,256)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 7        | 0.29          |
| (1,256)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 7        | 0.29          |
| (1,256)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 7        | 0.29          |
| (1,187)  | 1:98:A:SER:HB2   | 1:164:A:THR:HB   | 10       | 0.29          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 7        | 0.29          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 7        | 0.29          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 7        | 0.29          |
| (1,102)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HB3  | 1        | 0.29          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 2        | 0.29          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 2        | 0.29          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 2        | 0.29          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 8        | 0.29          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 8        | 0.29          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 8        | 0.29          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE1  | 1        | 0.28          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE2  | 1        | 0.28          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE1  | 2        | 0.28          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE2  | 2        | 0.28          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 3        | 0.28          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 7        | 0.28          |
| (1,3748) | 1:113:B:THR:H    | 1:112:B:LYS:HB2  | 3        | 0.28          |
| (1,3748) | 1:113:B:THR:H    | 1:112:B:LYS:HB2  | 9        | 0.28          |
| (1,3726) | 1:111:B:VAL:H    | 1:110:B:THR:HB   | 1        | 0.28          |
| (1,3726) | 1:111:B:VAL:H    | 1:110:B:THR:HB   | 6        | 0.28          |
| (1,3654) | 1:102:B:ASN:HD21 | 1:161:B:GLY:HA2  | 6        | 0.28          |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD21 | 5        | 0.28          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 4        | 0.28          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 4        | 0.28          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 4        | 0.28          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 1        | 0.28          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 1        | 0.28          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 1        | 0.28          |
| (1,3454) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB3  | 9        | 0.28          |
| (1,3454) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB3  | 9        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3454) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB3  | 9        | 0.28          |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 1        | 0.28          |
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 1        | 0.28          |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 1        | 0.28          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 2        | 0.28          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 3        | 0.28          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 8        | 0.28          |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 6        | 0.28          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 1        | 0.28          |
| (1,3211) | 1:144:B:LEU:HD11 | 1:148:B:VAL:HA   | 7        | 0.28          |
| (1,3211) | 1:144:B:LEU:HD12 | 1:148:B:VAL:HA   | 7        | 0.28          |
| (1,3211) | 1:144:B:LEU:HD13 | 1:148:B:VAL:HA   | 7        | 0.28          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG21 | 5        | 0.28          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG22 | 5        | 0.28          |
| (1,3201) | 1:144:B:LEU:HB3  | 1:148:B:VAL:HG23 | 5        | 0.28          |
| (1,3138) | 1:141:B:LYS:HG2  | 1:143:B:THR:HA   | 3        | 0.28          |
| (1,3137) | 1:141:B:LYS:HG2  | 1:142:B:TYR:HB3  | 3        | 0.28          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD1  | 9        | 0.28          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD2  | 9        | 0.28          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD1  | 9        | 0.28          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD2  | 9        | 0.28          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD1  | 9        | 0.28          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD2  | 9        | 0.28          |
| (1,3053) | 1:130:B:GLU:HA   | 1:130:B:GLU:HG2  | 4        | 0.28          |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 1        | 0.28          |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 5        | 0.28          |
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 9        | 0.28          |
| (1,2935) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HD2  | 2        | 0.28          |
| (1,2935) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HD2  | 2        | 0.28          |
| (1,2935) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HD2  | 2        | 0.28          |
| (1,2928) | 1:120:B:ILE:HG21 | 1:122:B:GLY:HA3  | 6        | 0.28          |
| (1,2928) | 1:120:B:ILE:HG22 | 1:122:B:GLY:HA3  | 6        | 0.28          |
| (1,2928) | 1:120:B:ILE:HG23 | 1:122:B:GLY:HA3  | 6        | 0.28          |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 4        | 0.28          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 1        | 0.28          |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 1        | 0.28          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 1        | 0.28          |
| (1,2738) | 1:112:B:LYS:HB2  | 1:120:B:ILE:HA   | 1        | 0.28          |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE3  | 5        | 0.28          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 5        | 0.28          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 5        | 0.28          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 5        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 2        | 0.28          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 2        | 0.28          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 2        | 0.28          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 5        | 0.28          |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 4        | 0.28          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 1        | 0.28          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 1        | 0.28          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 1        | 0.28          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 2        | 0.28          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 4        | 0.28          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 4        | 0.28          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 4        | 0.28          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 6        | 0.28          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 6        | 0.28          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 6        | 0.28          |
| (1,2353) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB3  | 5        | 0.28          |
| (1,2353) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB3  | 10       | 0.28          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 9        | 0.28          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 9        | 0.28          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 9        | 0.28          |
| (1,2318) | 1:94:B:ARG:HB2   | 1:96:B:ARG:HA    | 2        | 0.28          |
| (1,2282) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HA    | 5        | 0.28          |
| (1,2282) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HA    | 5        | 0.28          |
| (1,2282) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HA    | 5        | 0.28          |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 7        | 0.28          |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 7        | 0.28          |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 7        | 0.28          |
| (1,2207) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 9        | 0.28          |
| (1,2207) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 9        | 0.28          |
| (1,2207) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 9        | 0.28          |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 7        | 0.28          |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 7        | 0.28          |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 7        | 0.28          |
| (1,2075) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 9        | 0.28          |
| (1,2075) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 9        | 0.28          |
| (1,2075) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 9        | 0.28          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD2   | 10       | 0.28          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 8        | 0.28          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 3        | 0.28          |
| (1,1847) | 1:155:A:SER:H    | 1:154:A:SER:HB2  | 10       | 0.28          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 9        | 0.28          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 6        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 6        | 0.28          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 6        | 0.28          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 10       | 0.28          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 8        | 0.28          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 8        | 0.28          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 6        | 0.28          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 6        | 0.28          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 6        | 0.28          |
| (1,1323) | 1:94:A:ARG:H     | 1:93:A:ASP:HB3   | 6        | 0.28          |
| (1,1314) | 1:170:A:PRO:HB3  | 1:170:A:PRO:HD3  | 6        | 0.28          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 4        | 0.28          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 7        | 0.28          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 8        | 0.28          |
| (1,1280) | 1:168:A:PRO:HB2  | 1:170:A:PRO:HD3  | 2        | 0.28          |
| (1,1102) | 1:155:A:SER:HA   | 1:155:A:SER:HB3  | 7        | 0.28          |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 5        | 0.28          |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 6        | 0.28          |
| (1,990)  | 1:148:A:VAL:HA   | 1:169:A:MET:HB2  | 2        | 0.28          |
| (1,958)  | 1:145:A:PRO:HG3  | 1:146:A:PRO:HD2  | 6        | 0.28          |
| (1,845)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HD3  | 6        | 0.28          |
| (1,831)  | 1:139:A:THR:HB   | 1:141:A:LYS:HE2  | 8        | 0.28          |
| (1,826)  | 1:139:A:THR:HA   | 1:140:A:ARG:HB2  | 9        | 0.28          |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 6        | 0.28          |
| (1,687)  | 1:123:A:LYS:HB2  | 1:137:A:CYS:HB2  | 10       | 0.28          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG21 | 3        | 0.28          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG22 | 3        | 0.28          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG23 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 3        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 7        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 7        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 7        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 7        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 7        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 7        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 7        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 7        | 0.28          |
| (1,588)  | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 7        | 0.28          |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 4        | 0.28          |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 4        | 0.28          |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 4        | 0.28          |
| (1,427)  | 1:111:A:VAL:HG11 | 1:112:A:LYS:HE3  | 5        | 0.28          |
| (1,427)  | 1:111:A:VAL:HG12 | 1:112:A:LYS:HE3  | 5        | 0.28          |
| (1,427)  | 1:111:A:VAL:HG13 | 1:112:A:LYS:HE3  | 5        | 0.28          |
| (1,336)  | 1:108:A:GLU:HA   | 1:108:A:GLU:HG2  | 4        | 0.28          |
| (1,262)  | 1:100:A:ASP:HA   | 1:162:A:THR:HG21 | 6        | 0.28          |
| (1,262)  | 1:100:A:ASP:HA   | 1:162:A:THR:HG22 | 6        | 0.28          |
| (1,262)  | 1:100:A:ASP:HA   | 1:162:A:THR:HG23 | 6        | 0.28          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 10       | 0.28          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 10       | 0.28          |
| (1,232)  | 1:99:A:LEU:HD11  | 1:120:A:ILE:HG12 | 8        | 0.28          |
| (1,232)  | 1:99:A:LEU:HD12  | 1:120:A:ILE:HG12 | 8        | 0.28          |
| (1,232)  | 1:99:A:LEU:HD13  | 1:120:A:ILE:HG12 | 8        | 0.28          |
| (1,102)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HB3  | 7        | 0.28          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 5        | 0.28          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 5        | 0.28          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 5        | 0.28          |
| (1,9)    | 1:90:A:HIS:HB3   | 1:91:A:THR:HA    | 7        | 0.28          |
| (1,4263) | 1:167:B:ALA:H    | 1:166:B:GLU:HB3  | 6        | 0.27          |
| (1,4262) | 1:167:B:ALA:H    | 1:166:B:GLU:HB2  | 5        | 0.27          |
| (1,4025) | 1:148:B:VAL:H    | 1:146:B:PRO:HG2  | 4        | 0.27          |
| (1,3935) | 1:134:B:ILE:H    | 1:127:B:ARG:HB2  | 7        | 0.27          |
| (1,3902) | 1:129:B:ASP:H    | 1:129:B:ASP:HB2  | 8        | 0.27          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 1        | 0.27          |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 1        | 0.27          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD21 | 3        | 0.27          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD22 | 3        | 0.27          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD23 | 3        | 0.27          |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD21 | 3        | 0.27          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 10       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 10       | 0.27          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 10       | 0.27          |
| (1,3566) | 1:168:B:PRO:HD2  | 1:169:B:MET:HA   | 2        | 0.27          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 10       | 0.27          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 9        | 0.27          |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 1        | 0.27          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD21 | 7        | 0.27          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD22 | 7        | 0.27          |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD23 | 7        | 0.27          |
| (1,3395) | 1:155:B:SER:HB2  | 1:163:B:LEU:HA   | 5        | 0.27          |
| (1,3383) | 1:155:B:SER:HA   | 1:155:B:SER:HB3  | 10       | 0.27          |
| (1,3345) | 1:152:B:GLN:HB2  | 1:168:B:PRO:HD3  | 6        | 0.27          |
| (1,3274) | 1:148:B:VAL:HA   | 1:170:B:PRO:HG2  | 10       | 0.27          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 7        | 0.27          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 7        | 0.27          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 7        | 0.27          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 5        | 0.27          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 5        | 0.27          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 5        | 0.27          |
| (1,3092) | 1:136:B:ARG:HA   | 1:136:B:ARG:HG2  | 4        | 0.27          |
| (1,2975) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HA   | 10       | 0.27          |
| (1,2931) | 1:120:B:ILE:HG21 | 1:142:B:TYR:HD1  | 2        | 0.27          |
| (1,2931) | 1:120:B:ILE:HG21 | 1:142:B:TYR:HD2  | 2        | 0.27          |
| (1,2931) | 1:120:B:ILE:HG22 | 1:142:B:TYR:HD1  | 2        | 0.27          |
| (1,2931) | 1:120:B:ILE:HG22 | 1:142:B:TYR:HD2  | 2        | 0.27          |
| (1,2931) | 1:120:B:ILE:HG23 | 1:142:B:TYR:HD1  | 2        | 0.27          |
| (1,2931) | 1:120:B:ILE:HG23 | 1:142:B:TYR:HD2  | 2        | 0.27          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 1        | 0.27          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 1        | 0.27          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 1        | 0.27          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 9        | 0.27          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 9        | 0.27          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 9        | 0.27          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG21 | 7        | 0.27          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG22 | 7        | 0.27          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG23 | 7        | 0.27          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG21 | 9        | 0.27          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG22 | 9        | 0.27          |
| (1,2919) | 1:120:B:ILE:HG12 | 1:120:B:ILE:HG23 | 9        | 0.27          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD11 | 4        | 0.27          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD12 | 4        | 0.27          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD13 | 4        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 1        | 0.27          |
| (1,2625) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HD2  | 5        | 0.27          |
| (1,2619) | 1:108:B:GLU:HA   | 1:123:B:LYS:HD2  | 10       | 0.27          |
| (1,2613) | 1:107:B:ASP:HA   | 1:108:B:GLU:HG3  | 6        | 0.27          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 9        | 0.27          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 9        | 0.27          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 9        | 0.27          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 5        | 0.27          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 5        | 0.27          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 5        | 0.27          |
| (1,2332) | 1:95:B:TRP:HA    | 1:95:B:TRP:HB2   | 8        | 0.27          |
| (1,2313) | 1:94:B:ARG:HA    | 1:168:B:PRO:HD3  | 1        | 0.27          |
| (1,2287) | 1:90:B:HIS:HA    | 1:91:B:THR:HG21  | 8        | 0.27          |
| (1,2287) | 1:90:B:HIS:HA    | 1:91:B:THR:HG22  | 8        | 0.27          |
| (1,2287) | 1:90:B:HIS:HA    | 1:91:B:THR:HG23  | 8        | 0.27          |
| (1,2281) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 6        | 0.27          |
| (1,2213) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 6        | 0.27          |
| (1,2207) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 1        | 0.27          |
| (1,2207) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 1        | 0.27          |
| (1,2207) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 1        | 0.27          |
| (1,2192) | 1:134:B:ILE:HA   | 1:140:A:ARG:HG3  | 4        | 0.27          |
| (1,2152) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 5        | 0.27          |
| (1,2152) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 5        | 0.27          |
| (1,2152) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 5        | 0.27          |
| (1,2148) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 6        | 0.27          |
| (1,2081) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 6        | 0.27          |
| (1,2075) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HG2  | 1        | 0.27          |
| (1,2075) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HG2  | 1        | 0.27          |
| (1,2075) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HG2  | 1        | 0.27          |
| (1,2060) | 1:134:B:ILE:HA   | 1:140:A:ARG:HG3  | 4        | 0.27          |
| (1,2020) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 5        | 0.27          |
| (1,2020) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 5        | 0.27          |
| (1,2020) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 5        | 0.27          |
| (1,2009) | 1:171:A:LYS:H    | 1:171:A:LYS:HB2  | 6        | 0.27          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 9        | 0.27          |
| (1,1703) | 1:142:A:TYR:H    | 1:141:A:LYS:HG3  | 1        | 0.27          |
| (1,1703) | 1:142:A:TYR:H    | 1:141:A:LYS:HG3  | 7        | 0.27          |
| (1,1626) | 1:129:A:ASP:H    | 1:132:A:GLY:HA3  | 9        | 0.27          |
| (1,1584) | 1:125:A:GLU:H    | 1:126:A:GLU:H    | 2        | 0.27          |
| (1,1580) | 1:125:A:GLU:H    | 1:108:A:GLU:HG2  | 7        | 0.27          |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 3        | 0.27          |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 4        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 1        | 0.27          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 1        | 0.27          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 5        | 0.27          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD11 | 8        | 0.27          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD12 | 8        | 0.27          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD13 | 8        | 0.27          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 7        | 0.27          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 7        | 0.27          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 7        | 0.27          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 6        | 0.27          |
| (1,1191) | 1:158:A:SER:HB2  | 1:160:A:GLU:HG2  | 6        | 0.27          |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 9        | 0.27          |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 3        | 0.27          |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 3        | 0.27          |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 3        | 0.27          |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 6        | 0.27          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 10       | 0.27          |
| (1,917)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA2  | 1        | 0.27          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 2        | 0.27          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 2        | 0.27          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 2        | 0.27          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 7        | 0.27          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 7        | 0.27          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 7        | 0.27          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 5        | 0.27          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 5        | 0.27          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 5        | 0.27          |
| (1,837)  | 1:140:A:ARG:HA   | 1:140:A:ARG:HD3  | 8        | 0.27          |
| (1,808)  | 1:135:A:SER:HA   | 1:135:A:SER:HB2  | 2        | 0.27          |
| (1,782)  | 1:131:A:HIS:HB2  | 1:132:A:GLY:HA2  | 8        | 0.27          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 1        | 0.27          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 8        | 0.27          |
| (1,715)  | 1:126:A:GLU:HB2  | 1:135:A:SER:HB3  | 9        | 0.27          |
| (1,689)  | 1:123:A:LYS:HB3  | 1:137:A:CYS:HA   | 8        | 0.27          |
| (1,647)  | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 3        | 0.27          |
| (1,647)  | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 3        | 0.27          |
| (1,647)  | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 3        | 0.27          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 5        | 0.27          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 5        | 0.27          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 5        | 0.27          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 10       | 0.27          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 10       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 10       | 0.27          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG21 | 5        | 0.27          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG22 | 5        | 0.27          |
| (1,638)  | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG23 | 5        | 0.27          |
| (1,455)  | 1:112:A:LYS:HB2  | 1:112:A:LYS:HE3  | 9        | 0.27          |
| (1,453)  | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 8        | 0.27          |
| (1,359)  | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 6        | 0.27          |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 9        | 0.27          |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 9        | 0.27          |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 9        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 8        | 0.27          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 8        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG11 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG12 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG13 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG11 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG12 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG13 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG11 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG12 | 2        | 0.27          |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG13 | 2        | 0.27          |
| (1,99)   | 1:96:A:ARG:HB3   | 1:164:A:THR:HB   | 10       | 0.27          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 4        | 0.27          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 4        | 0.27          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 4        | 0.27          |
| (1,72)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB3  | 6        | 0.27          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 7        | 0.27          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 7        | 0.27          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 7        | 0.27          |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 4        | 0.27          |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 1        | 0.26          |
| (1,3915) | 1:131:B:HIS:H    | 1:129:B:ASP:HB3  | 9        | 0.26          |
| (1,3907) | 1:129:B:ASP:H    | 1:132:B:GLY:HA3  | 3        | 0.26          |
| (1,3862) | 1:125:B:GLU:H    | 1:108:B:GLU:HG3  | 5        | 0.26          |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 9        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 10       | 0.26          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 3        | 0.26          |
| (1,3672) | 1:105:B:ALA:H    | 1:108:B:GLU:HB3  | 2        | 0.26          |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD21 | 8        | 0.26          |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD22 | 8        | 0.26          |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD23 | 8        | 0.26          |
| (1,3602) | 1:94:B:ARG:H     | 1:93:B:ASP:HA    | 9        | 0.26          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG21  | 1        | 0.26          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG22  | 1        | 0.26          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG23  | 1        | 0.26          |
| (1,3595) | 1:170:B:PRO:HB3  | 1:170:B:PRO:HD3  | 9        | 0.26          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD11 | 1        | 0.26          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD12 | 1        | 0.26          |
| (1,3437) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HD13 | 1        | 0.26          |
| (1,3346) | 1:152:B:GLN:HB2  | 1:169:B:MET:HA   | 5        | 0.26          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 9        | 0.26          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 9        | 0.26          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 9        | 0.26          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 10       | 0.26          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 10       | 0.26          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 10       | 0.26          |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 1        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 1        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 1        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 3        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 3        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 3        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 9        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 9        | 0.26          |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 9        | 0.26          |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 3        | 0.26          |
| (1,3096) | 1:136:B:ARG:HG3  | 1:138:B:PHE:HA   | 8        | 0.26          |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 3        | 0.26          |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 5        | 0.26          |
| (1,3054) | 1:130:B:GLU:HA   | 1:130:B:GLU:HG3  | 3        | 0.26          |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 3        | 0.26          |
| (1,2930) | 1:120:B:ILE:HG21 | 1:140:B:ARG:HA   | 3        | 0.26          |
| (1,2930) | 1:120:B:ILE:HG22 | 1:140:B:ARG:HA   | 3        | 0.26          |
| (1,2930) | 1:120:B:ILE:HG23 | 1:140:B:ARG:HA   | 3        | 0.26          |
| (1,2929) | 1:120:B:ILE:HG21 | 1:139:B:THR:HA   | 1        | 0.26          |
| (1,2929) | 1:120:B:ILE:HG22 | 1:139:B:THR:HA   | 1        | 0.26          |
| (1,2929) | 1:120:B:ILE:HG23 | 1:139:B:THR:HA   | 1        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 9        | 0.26          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 4        | 0.26          |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 4        | 0.26          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 4        | 0.26          |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE3  | 1        | 0.26          |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE3  | 1        | 0.26          |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE3  | 1        | 0.26          |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE3  | 8        | 0.26          |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE3  | 8        | 0.26          |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE3  | 8        | 0.26          |
| (1,2686) | 1:110:B:THR:HG21 | 1:112:B:LYS:HD3  | 2        | 0.26          |
| (1,2686) | 1:110:B:THR:HG22 | 1:112:B:LYS:HD3  | 2        | 0.26          |
| (1,2686) | 1:110:B:THR:HG23 | 1:112:B:LYS:HD3  | 2        | 0.26          |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 4        | 0.26          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 6        | 0.26          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 9        | 0.26          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 9        | 0.26          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 9        | 0.26          |
| (1,2625) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HD2  | 1        | 0.26          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD21 | 8        | 0.26          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD22 | 8        | 0.26          |
| (1,2616) | 1:107:B:ASP:HA   | 1:157:B:LEU:HD23 | 8        | 0.26          |
| (1,2592) | 1:106:B:PRO:HA   | 1:109:B:LEU:HB2  | 10       | 0.26          |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 1        | 0.26          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 4        | 0.26          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 4        | 0.26          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 4        | 0.26          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG21  | 1        | 0.26          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG22  | 1        | 0.26          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG23  | 1        | 0.26          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 2        | 0.26          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 2        | 0.26          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 2        | 0.26          |
| (1,2352) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB2  | 4        | 0.26          |
| (1,2326) | 1:94:B:ARG:HG2   | 1:168:B:PRO:HB2  | 4        | 0.26          |
| (1,2283) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HB3   | 3        | 0.26          |
| (1,2283) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HB3   | 3        | 0.26          |
| (1,2283) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HB3   | 3        | 0.26          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 3        | 0.26          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 3        | 0.26          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 3        | 0.26          |
| (1,2169) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 5        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2152) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 9        | 0.26          |
| (1,2152) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 9        | 0.26          |
| (1,2152) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 9        | 0.26          |
| (1,2150) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB3  | 3        | 0.26          |
| (1,2150) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB3  | 3        | 0.26          |
| (1,2150) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB3  | 3        | 0.26          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 3        | 0.26          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 3        | 0.26          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 3        | 0.26          |
| (1,2037) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 5        | 0.26          |
| (1,2020) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 9        | 0.26          |
| (1,2020) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 9        | 0.26          |
| (1,2020) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 9        | 0.26          |
| (1,2018) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB3  | 3        | 0.26          |
| (1,2018) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB3  | 3        | 0.26          |
| (1,2018) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB3  | 3        | 0.26          |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD11 | 8        | 0.26          |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD12 | 8        | 0.26          |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD13 | 8        | 0.26          |
| (1,1915) | 1:162:A:THR:H    | 1:102:A:ASN:HB2  | 8        | 0.26          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG21 | 5        | 0.26          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG22 | 5        | 0.26          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG23 | 5        | 0.26          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 5        | 0.26          |
| (1,1626) | 1:129:A:ASP:H    | 1:132:A:GLY:HA3  | 7        | 0.26          |
| (1,1598) | 1:128:A:GLN:H    | 1:127:A:ARG:HG2  | 3        | 0.26          |
| (1,1525) | 1:119:A:GLU:H    | 1:114:A:LYS:HB3  | 3        | 0.26          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 7        | 0.26          |
| (1,1459) | 1:112:A:LYS:H    | 1:112:A:LYS:HE3  | 1        | 0.26          |
| (1,1408) | 1:107:A:ASP:H    | 1:157:A:LEU:HD12 | 10       | 0.26          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 2        | 0.26          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 3        | 0.26          |
| (1,1399) | 1:107:A:ASP:H    | 1:106:A:PRO:HB2  | 10       | 0.26          |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 9        | 0.26          |
| (1,1302) | 1:169:A:MET:HB2  | 1:171:A:LYS:HE3  | 2        | 0.26          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 2        | 0.26          |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 5        | 0.26          |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 4        | 0.26          |
| (1,1179) | 1:157:A:LEU:HD21 | 1:163:A:LEU:HB3  | 9        | 0.26          |
| (1,1179) | 1:157:A:LEU:HD22 | 1:163:A:LEU:HB3  | 9        | 0.26          |
| (1,1179) | 1:157:A:LEU:HD23 | 1:163:A:LEU:HB3  | 9        | 0.26          |
| (1,1179) | 1:157:A:LEU:HD21 | 1:163:A:LEU:HB3  | 10       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1179) | 1:157:A:LEU:HD22 | 1:163:A:LEU:HB3  | 10       | 0.26          |
| (1,1179) | 1:157:A:LEU:HD23 | 1:163:A:LEU:HB3  | 10       | 0.26          |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 5        | 0.26          |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 5        | 0.26          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 5        | 0.26          |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 1        | 0.26          |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 1        | 0.26          |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 1        | 0.26          |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 10       | 0.26          |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 10       | 0.26          |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 10       | 0.26          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD11 | 3        | 0.26          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD12 | 3        | 0.26          |
| (1,1156) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HD13 | 3        | 0.26          |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 8        | 0.26          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 1        | 0.26          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 4        | 0.26          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 6        | 0.26          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 9        | 0.26          |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG11 | 6        | 0.26          |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG12 | 6        | 0.26          |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG13 | 6        | 0.26          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 10       | 0.26          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 10       | 0.26          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 10       | 0.26          |
| (1,842)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 5        | 0.26          |
| (1,831)  | 1:139:A:THR:HB   | 1:141:A:LYS:HE2  | 6        | 0.26          |
| (1,808)  | 1:135:A:SER:HA   | 1:135:A:SER:HB2  | 3        | 0.26          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 8        | 0.26          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 8        | 0.26          |
| (1,641)  | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 8        | 0.26          |
| (1,639)  | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 10       | 0.26          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 10       | 0.26          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 10       | 0.26          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 10       | 0.26          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 10       | 0.26          |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 10       | 0.26          |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 10       | 0.26          |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 4        | 0.26          |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 4        | 0.26          |
| (1,529)  | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 4        | 0.26          |
| (1,478)  | 1:112:A:LYS:HE2  | 1:121:A:THR:HB   | 7        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,359)  | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 2        | 0.26          |
| (1,347)  | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD2  | 4        | 0.26          |
| (1,337)  | 1:108:A:GLU:HA   | 1:108:A:GLU:HG3  | 6        | 0.26          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD11 | 4        | 0.26          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD12 | 4        | 0.26          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD13 | 4        | 0.26          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD11 | 7        | 0.26          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD12 | 7        | 0.26          |
| (1,276)  | 1:102:A:ASN:HB2  | 1:157:A:LEU:HD13 | 7        | 0.26          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 7        | 0.26          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 7        | 0.26          |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 7        | 0.26          |
| (1,166)  | 1:97:A:VAL:HG21  | 1:118:A:VAL:HB   | 2        | 0.26          |
| (1,166)  | 1:97:A:VAL:HG22  | 1:118:A:VAL:HB   | 2        | 0.26          |
| (1,166)  | 1:97:A:VAL:HG23  | 1:118:A:VAL:HB   | 2        | 0.26          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 9        | 0.26          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 9        | 0.26          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 9        | 0.26          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 5        | 0.26          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 5        | 0.26          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 5        | 0.26          |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 7        | 0.26          |
| (1,18)   | 1:93:A:ASP:HB2   | 1:94:A:ARG:HA    | 3        | 0.26          |
| (1,9)    | 1:90:A:HIS:HB3   | 1:91:A:THR:HA    | 5        | 0.26          |
| (1,4281) | 1:169:B:MET:H    | 1:169:B:MET:HG3  | 8        | 0.25          |
| (1,4279) | 1:169:B:MET:H    | 1:169:B:MET:HB2  | 9        | 0.25          |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 1        | 0.25          |
| (1,4048) | 1:149:B:ASP:H    | 1:170:B:PRO:HG3  | 10       | 0.25          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD21  | 3        | 0.25          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD22  | 3        | 0.25          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD23  | 3        | 0.25          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD21  | 9        | 0.25          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD22  | 9        | 0.25          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD23  | 9        | 0.25          |
| (1,3936) | 1:134:B:ILE:H    | 1:127:B:ARG:HG2  | 8        | 0.25          |
| (1,3908) | 1:129:B:ASP:H    | 1:132:B:GLY:H    | 4        | 0.25          |
| (1,3904) | 1:129:B:ASP:H    | 1:130:B:GLU:HG3  | 10       | 0.25          |
| (1,3896) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HB3  | 1        | 0.25          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD1  | 6        | 0.25          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD2  | 6        | 0.25          |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 8        | 0.25          |
| (1,3748) | 1:113:B:THR:H    | 1:112:B:LYS:HB2  | 7        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD11 | 10       | 0.25          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD12 | 10       | 0.25          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD13 | 10       | 0.25          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD21 | 7        | 0.25          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD22 | 7        | 0.25          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD23 | 7        | 0.25          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD11 | 7        | 0.25          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD12 | 7        | 0.25          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD13 | 7        | 0.25          |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD22 | 8        | 0.25          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 6        | 0.25          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 6        | 0.25          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 6        | 0.25          |
| (1,3605) | 1:94:B:ARG:H     | 1:94:B:ARG:HG3   | 7        | 0.25          |
| (1,3604) | 1:94:B:ARG:H     | 1:93:B:ASP:HB3   | 2        | 0.25          |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 8        | 0.25          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 1        | 0.25          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 6        | 0.25          |
| (1,3302) | 1:148:B:VAL:HG21 | 1:169:B:MET:HB3  | 3        | 0.25          |
| (1,3302) | 1:148:B:VAL:HG22 | 1:169:B:MET:HB3  | 3        | 0.25          |
| (1,3302) | 1:148:B:VAL:HG23 | 1:169:B:MET:HB3  | 3        | 0.25          |
| (1,3302) | 1:148:B:VAL:HG21 | 1:169:B:MET:HB3  | 10       | 0.25          |
| (1,3302) | 1:148:B:VAL:HG22 | 1:169:B:MET:HB3  | 10       | 0.25          |
| (1,3302) | 1:148:B:VAL:HG23 | 1:169:B:MET:HB3  | 10       | 0.25          |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 2        | 0.25          |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 2        | 0.25          |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 2        | 0.25          |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 10       | 0.25          |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 10       | 0.25          |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 10       | 0.25          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 1        | 0.25          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG2  | 2        | 0.25          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 8        | 0.25          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 10       | 0.25          |
| (1,3164) | 1:142:B:TYR:HD1  | 1:165:B:VAL:HG21 | 2        | 0.25          |
| (1,3164) | 1:142:B:TYR:HD1  | 1:165:B:VAL:HG22 | 2        | 0.25          |
| (1,3164) | 1:142:B:TYR:HD1  | 1:165:B:VAL:HG23 | 2        | 0.25          |
| (1,3164) | 1:142:B:TYR:HD2  | 1:165:B:VAL:HG21 | 2        | 0.25          |
| (1,3164) | 1:142:B:TYR:HD2  | 1:165:B:VAL:HG22 | 2        | 0.25          |
| (1,3164) | 1:142:B:TYR:HD2  | 1:165:B:VAL:HG23 | 2        | 0.25          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD1  | 2        | 0.25          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD2  | 2        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD1  | 2        | 0.25          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD2  | 2        | 0.25          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD1  | 2        | 0.25          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD2  | 2        | 0.25          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 1        | 0.25          |
| (1,3058) | 1:131:B:HIS:HA   | 1:131:B:HIS:HB3  | 4        | 0.25          |
| (1,2968) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB2  | 4        | 0.25          |
| (1,2965) | 1:123:B:LYS:HA   | 1:135:B:SER:HB3  | 10       | 0.25          |
| (1,2935) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HD2  | 5        | 0.25          |
| (1,2935) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HD2  | 5        | 0.25          |
| (1,2935) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HD2  | 5        | 0.25          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 7        | 0.25          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 7        | 0.25          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 7        | 0.25          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 1        | 0.25          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 1        | 0.25          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 1        | 0.25          |
| (1,2716) | 1:111:B:VAL:HG11 | 1:120:B:ILE:HG13 | 10       | 0.25          |
| (1,2716) | 1:111:B:VAL:HG12 | 1:120:B:ILE:HG13 | 10       | 0.25          |
| (1,2716) | 1:111:B:VAL:HG13 | 1:120:B:ILE:HG13 | 10       | 0.25          |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE3  | 7        | 0.25          |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE3  | 7        | 0.25          |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE3  | 7        | 0.25          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 7        | 0.25          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 7        | 0.25          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 7        | 0.25          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 10       | 0.25          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 10       | 0.25          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 1        | 0.25          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 1        | 0.25          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 1        | 0.25          |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD2  | 7        | 0.25          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 2        | 0.25          |
| (1,2605) | 1:106:B:PRO:HB3  | 1:107:B:ASP:HA   | 10       | 0.25          |
| (1,2568) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB3  | 5        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 5        | 0.25          |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 8        | 0.25          |
| (1,2529) | 1:99:B:LEU:HD21  | 1:140:B:ARG:HD2  | 8        | 0.25          |
| (1,2529) | 1:99:B:LEU:HD22  | 1:140:B:ARG:HD2  | 8        | 0.25          |
| (1,2529) | 1:99:B:LEU:HD23  | 1:140:B:ARG:HD2  | 8        | 0.25          |
| (1,2393) | 1:96:B:ARG:HD3   | 1:164:B:THR:HA   | 1        | 0.25          |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 1        | 0.25          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 4        | 0.25          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 1        | 0.25          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 1        | 0.25          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 1        | 0.25          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 10       | 0.25          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 10       | 0.25          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 10       | 0.25          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 7        | 0.25          |
| (1,2353) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB3  | 1        | 0.25          |
| (1,2353) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB3  | 6        | 0.25          |
| (1,2352) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB2  | 6        | 0.25          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 4        | 0.25          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 4        | 0.25          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 4        | 0.25          |
| (1,2326) | 1:94:B:ARG:HG2   | 1:168:B:PRO:HB2  | 9        | 0.25          |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 2        | 0.25          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 9        | 0.25          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 9        | 0.25          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 9        | 0.25          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 1        | 0.25          |
| (1,2185) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 2        | 0.25          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 9        | 0.25          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 9        | 0.25          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 9        | 0.25          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 1        | 0.25          |
| (1,2053) | 1:133:A:TYR:HB3  | 1:141:B:LYS:HD2  | 2        | 0.25          |
| (1,2015) | 1:173:A:ALA:H    | 1:172:A:LEU:HG   | 9        | 0.25          |
| (1,1910) | 1:161:A:GLY:H    | 1:160:A:GLU:HG3  | 2        | 0.25          |
| (1,1654) | 1:134:A:ILE:H    | 1:127:A:ARG:HB2  | 4        | 0.25          |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG2  | 5        | 0.25          |
| (1,1634) | 1:131:A:HIS:H    | 1:129:A:ASP:HB3  | 1        | 0.25          |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD1  | 10       | 0.25          |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD2  | 10       | 0.25          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB1  | 6        | 0.25          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB2  | 6        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB3  | 6        | 0.25          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 3        | 0.25          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 3        | 0.25          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 3        | 0.25          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 6        | 0.25          |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD12 | 9        | 0.25          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD21 | 5        | 0.25          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD22 | 5        | 0.25          |
| (1,1372) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD23 | 5        | 0.25          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG21 | 1        | 0.25          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG22 | 1        | 0.25          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG23 | 1        | 0.25          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG21 | 3        | 0.25          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG22 | 3        | 0.25          |
| (1,1344) | 1:97:A:VAL:H     | 1:165:A:VAL:HG23 | 3        | 0.25          |
| (1,1327) | 1:94:A:ARG:H     | 1:169:A:MET:HG2  | 6        | 0.25          |
| (1,1210) | 1:160:A:GLU:HB2  | 1:162:A:THR:HB   | 9        | 0.25          |
| (1,1173) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB3  | 9        | 0.25          |
| (1,1173) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB3  | 9        | 0.25          |
| (1,1173) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB3  | 9        | 0.25          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 3        | 0.25          |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 3        | 0.25          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 3        | 0.25          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 10       | 0.25          |
| (1,862)  | 1:141:A:LYS:HG3  | 1:142:A:TYR:HB3  | 1        | 0.25          |
| (1,827)  | 1:139:A:THR:HA   | 1:140:A:ARG:HG2  | 1        | 0.25          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD1  | 7        | 0.25          |
| (1,797)  | 1:134:A:ILE:HG21 | 1:133:A:TYR:HD2  | 7        | 0.25          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD1  | 7        | 0.25          |
| (1,797)  | 1:134:A:ILE:HG22 | 1:133:A:TYR:HD2  | 7        | 0.25          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD1  | 7        | 0.25          |
| (1,797)  | 1:134:A:ILE:HG23 | 1:133:A:TYR:HD2  | 7        | 0.25          |
| (1,749)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HE1  | 5        | 0.25          |
| (1,749)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HE2  | 5        | 0.25          |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG23 | 3        | 0.25          |
| (1,716)  | 1:126:A:GLU:HG2  | 1:127:A:ARG:HG2  | 2        | 0.25          |
| (1,701)  | 1:125:A:GLU:HA   | 1:126:A:GLU:HG2  | 9        | 0.25          |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 6        | 0.25          |
| (1,671)  | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 5        | 0.25          |
| (1,671)  | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 5        | 0.25          |
| (1,671)  | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 5        | 0.25          |
| (1,649)  | 1:120:A:ILE:HG21 | 1:140:A:ARG:HA   | 7        | 0.25          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,649) | 1:120:A:ILE:HG22 | 1:140:A:ARG:HA   | 7        | 0.25          |
| (1,649) | 1:120:A:ILE:HG23 | 1:140:A:ARG:HA   | 7        | 0.25          |
| (1,641) | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 1        | 0.25          |
| (1,641) | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 1        | 0.25          |
| (1,641) | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 1        | 0.25          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 5        | 0.25          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 5        | 0.25          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 2        | 0.25          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 2        | 0.25          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 2        | 0.25          |
| (1,434) | 1:111:A:VAL:HG11 | 1:120:A:ILE:HG12 | 4        | 0.25          |
| (1,434) | 1:111:A:VAL:HG12 | 1:120:A:ILE:HG12 | 4        | 0.25          |
| (1,434) | 1:111:A:VAL:HG13 | 1:120:A:ILE:HG12 | 4        | 0.25          |
| (1,418) | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 10       | 0.25          |
| (1,405) | 1:110:A:THR:HG21 | 1:112:A:LYS:HD3  | 10       | 0.25          |
| (1,405) | 1:110:A:THR:HG22 | 1:112:A:LYS:HD3  | 10       | 0.25          |
| (1,405) | 1:110:A:THR:HG23 | 1:112:A:LYS:HD3  | 10       | 0.25          |
| (1,383) | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 7        | 0.25          |
| (1,383) | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 7        | 0.25          |
| (1,383) | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 7        | 0.25          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD11 | 1        | 0.25          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD12 | 1        | 0.25          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD13 | 1        | 0.25          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 6        | 0.25          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 6        | 0.25          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 6        | 0.25          |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 4        | 0.25          |
| (1,344) | 1:108:A:GLU:HG2  | 1:123:A:LYS:HD3  | 1        | 0.25          |
| (1,344) | 1:108:A:GLU:HG2  | 1:123:A:LYS:HD2  | 3        | 0.25          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 1        | 0.25          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 1        | 0.25          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 1        | 0.25          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 7        | 0.25          |
| (1,226) | 1:99:A:LEU:HD11  | 1:101:A:VAL:HG21 | 2        | 0.25          |
| (1,226) | 1:99:A:LEU:HD11  | 1:101:A:VAL:HG22 | 2        | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,226)  | 1:99:A:LEU:HD11 | 1:101:A:VAL:HG23 | 2        | 0.25          |
| (1,226)  | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG21 | 2        | 0.25          |
| (1,226)  | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG22 | 2        | 0.25          |
| (1,226)  | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG23 | 2        | 0.25          |
| (1,226)  | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG21 | 2        | 0.25          |
| (1,226)  | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG22 | 2        | 0.25          |
| (1,226)  | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG23 | 2        | 0.25          |
| (1,187)  | 1:98:A:SER:HB2  | 1:164:A:THR:HB   | 2        | 0.25          |
| (1,155)  | 1:97:A:VAL:HG21 | 1:144:A:LEU:HB2  | 10       | 0.25          |
| (1,155)  | 1:97:A:VAL:HG22 | 1:144:A:LEU:HB2  | 10       | 0.25          |
| (1,155)  | 1:97:A:VAL:HG23 | 1:144:A:LEU:HB2  | 10       | 0.25          |
| (1,102)  | 1:96:A:ARG:HB3  | 1:166:A:GLU:HB3  | 5        | 0.25          |
| (1,72)   | 1:95:A:TRP:HB2  | 1:168:A:PRO:HB3  | 8        | 0.25          |
| (1,19)   | 1:93:A:ASP:HB2  | 1:94:A:ARG:HG2   | 7        | 0.25          |
| (1,4262) | 1:167:B:ALA:H   | 1:166:B:GLU:HB2  | 10       | 0.24          |
| (1,4259) | 1:167:B:ALA:H   | 1:96:B:ARG:HD2   | 5        | 0.24          |
| (1,4168) | 1:158:B:SER:H   | 1:162:B:THR:HG21 | 1        | 0.24          |
| (1,4168) | 1:158:B:SER:H   | 1:162:B:THR:HG22 | 1        | 0.24          |
| (1,4168) | 1:158:B:SER:H   | 1:162:B:THR:HG23 | 1        | 0.24          |
| (1,4128) | 1:155:B:SER:H   | 1:154:B:SER:HB2  | 3        | 0.24          |
| (1,3925) | 1:132:B:GLY:H   | 1:130:B:GLU:HG3  | 10       | 0.24          |
| (1,3918) | 1:131:B:HIS:H   | 1:130:B:GLU:HG3  | 6        | 0.24          |
| (1,3910) | 1:129:B:ASP:H   | 1:133:B:TYR:HB2  | 1        | 0.24          |
| (1,3904) | 1:129:B:ASP:H   | 1:130:B:GLU:HG2  | 4        | 0.24          |
| (1,3865) | 1:125:B:GLU:H   | 1:126:B:GLU:H    | 4        | 0.24          |
| (1,3865) | 1:125:B:GLU:H   | 1:126:B:GLU:H    | 9        | 0.24          |
| (1,3848) | 1:123:B:LYS:H   | 1:109:B:LEU:HG   | 4        | 0.24          |
| (1,3798) | 1:118:B:VAL:H   | 1:142:B:TYR:HB2  | 9        | 0.24          |
| (1,3726) | 1:111:B:VAL:H   | 1:110:B:THR:HB   | 10       | 0.24          |
| (1,3681) | 1:107:B:ASP:H   | 1:106:B:PRO:HB3  | 6        | 0.24          |
| (1,3500) | 1:162:B:THR:HA  | 1:162:B:THR:HG21 | 1        | 0.24          |
| (1,3500) | 1:162:B:THR:HA  | 1:162:B:THR:HG22 | 1        | 0.24          |
| (1,3500) | 1:162:B:THR:HA  | 1:162:B:THR:HG23 | 1        | 0.24          |
| (1,3470) | 1:158:B:SER:HA  | 1:160:B:GLU:HB3  | 1        | 0.24          |
| (1,3422) | 1:156:B:SER:HB3 | 1:163:B:LEU:HD21 | 4        | 0.24          |
| (1,3422) | 1:156:B:SER:HB3 | 1:163:B:LEU:HD22 | 4        | 0.24          |
| (1,3422) | 1:156:B:SER:HB3 | 1:163:B:LEU:HD23 | 4        | 0.24          |
| (1,3381) | 1:154:B:SER:HB2 | 1:165:B:VAL:HG21 | 2        | 0.24          |
| (1,3381) | 1:154:B:SER:HB2 | 1:165:B:VAL:HG22 | 2        | 0.24          |
| (1,3381) | 1:154:B:SER:HB2 | 1:165:B:VAL:HG23 | 2        | 0.24          |
| (1,3309) | 1:149:B:ASP:HA  | 1:150:B:PRO:HD3  | 1        | 0.24          |
| (1,3138) | 1:141:B:LYS:HG2 | 1:143:B:THR:HA   | 4        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 6        | 0.24          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 3        | 0.24          |
| (1,3004) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB2  | 8        | 0.24          |
| (1,2991) | 1:126:B:GLU:HA   | 1:135:B:SER:HB2  | 8        | 0.24          |
| (1,2975) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HA   | 2        | 0.24          |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE1  | 9        | 0.24          |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE2  | 9        | 0.24          |
| (1,2894) | 1:119:B:GLU:HB3  | 1:121:B:THR:HB   | 8        | 0.24          |
| (1,2738) | 1:112:B:LYS:HB2  | 1:120:B:ILE:HA   | 10       | 0.24          |
| (1,2686) | 1:110:B:THR:HG21 | 1:112:B:LYS:HD3  | 5        | 0.24          |
| (1,2686) | 1:110:B:THR:HG22 | 1:112:B:LYS:HD3  | 5        | 0.24          |
| (1,2686) | 1:110:B:THR:HG23 | 1:112:B:LYS:HD3  | 5        | 0.24          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 6        | 0.24          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 6        | 0.24          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 6        | 0.24          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD11 | 9        | 0.24          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD12 | 9        | 0.24          |
| (1,2645) | 1:109:B:LEU:HG   | 1:120:B:ILE:HD13 | 9        | 0.24          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 6        | 0.24          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 6        | 0.24          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 6        | 0.24          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 10       | 0.24          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 10       | 0.24          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 10       | 0.24          |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 3        | 0.24          |
| (1,2617) | 1:108:B:GLU:HA   | 1:108:B:GLU:HG2  | 4        | 0.24          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 2        | 0.24          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 2        | 0.24          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 2        | 0.24          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 5        | 0.24          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 5        | 0.24          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 5        | 0.24          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 7        | 0.24          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 7        | 0.24          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 7        | 0.24          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG21  | 5        | 0.24          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG22  | 5        | 0.24          |
| (1,2364) | 1:96:B:ARG:HA    | 1:97:B:VAL:HG23  | 5        | 0.24          |
| (1,2322) | 1:94:B:ARG:HB3   | 1:167:B:ALA:HA   | 9        | 0.24          |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 1        | 0.24          |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 1        | 0.24          |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 1        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2215) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 5        | 0.24          |
| (1,2215) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 9        | 0.24          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 5        | 0.24          |
| (1,2192) | 1:134:B:ILE:HA   | 1:140:A:ARG:HG3  | 3        | 0.24          |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 1        | 0.24          |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 1        | 0.24          |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 1        | 0.24          |
| (1,2083) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 5        | 0.24          |
| (1,2083) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 9        | 0.24          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 5        | 0.24          |
| (1,2060) | 1:134:B:ILE:HA   | 1:140:A:ARG:HG3  | 3        | 0.24          |
| (1,2007) | 1:171:A:LYS:H    | 1:170:A:PRO:HD3  | 6        | 0.24          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 6        | 0.24          |
| (1,1978) | 1:167:A:ALA:H    | 1:96:A:ARG:HD3   | 1        | 0.24          |
| (1,1884) | 1:158:A:SER:H    | 1:158:A:SER:HB3  | 2        | 0.24          |
| (1,1805) | 1:152:A:GLN:HE21 | 1:170:A:PRO:HD3  | 8        | 0.24          |
| (1,1796) | 1:152:A:GLN:HE21 | 1:149:A:ASP:HB2  | 4        | 0.24          |
| (1,1796) | 1:152:A:GLN:HE21 | 1:149:A:ASP:HB2  | 8        | 0.24          |
| (1,1657) | 1:134:A:ILE:H    | 1:133:A:TYR:HB3  | 4        | 0.24          |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD1  | 2        | 0.24          |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD2  | 2        | 0.24          |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 2        | 0.24          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 4        | 0.24          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD21 | 6        | 0.24          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD21 | 9        | 0.24          |
| (1,1280) | 1:168:A:PRO:HB2  | 1:170:A:PRO:HD3  | 7        | 0.24          |
| (1,1211) | 1:160:A:GLU:HG2  | 1:162:A:THR:HB   | 2        | 0.24          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 5        | 0.24          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD21 | 1        | 0.24          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD22 | 1        | 0.24          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD23 | 1        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD21 | 1        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD22 | 1        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD23 | 1        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD21 | 6        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD22 | 6        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD23 | 6        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD21 | 8        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD22 | 8        | 0.24          |
| (1,1122) | 1:155:A:SER:HB3  | 1:157:A:LEU:HD23 | 8        | 0.24          |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 8        | 0.24          |
| (1,1065) | 1:152:A:GLN:HB2  | 1:169:A:MET:HA   | 8        | 0.24          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 2        | 0.24          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 2        | 0.24          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 2        | 0.24          |
| (1,862) | 1:141:A:LYS:HG3  | 1:142:A:TYR:HB3  | 9        | 0.24          |
| (1,858) | 1:141:A:LYS:HG3  | 1:141:A:LYS:HE2  | 5        | 0.24          |
| (1,754) | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE1  | 5        | 0.24          |
| (1,754) | 1:128:A:GLN:HB2  | 1:133:A:TYR:HE2  | 5        | 0.24          |
| (1,671) | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 7        | 0.24          |
| (1,671) | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 7        | 0.24          |
| (1,671) | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 7        | 0.24          |
| (1,654) | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD2  | 7        | 0.24          |
| (1,654) | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD2  | 7        | 0.24          |
| (1,654) | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD2  | 7        | 0.24          |
| (1,638) | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG21 | 8        | 0.24          |
| (1,638) | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG22 | 8        | 0.24          |
| (1,638) | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG23 | 8        | 0.24          |
| (1,638) | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG21 | 10       | 0.24          |
| (1,638) | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG22 | 10       | 0.24          |
| (1,638) | 1:120:A:ILE:HG12 | 1:120:A:ILE:HG23 | 10       | 0.24          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 2        | 0.24          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 8        | 0.24          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 8        | 0.24          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 1        | 0.24          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 1        | 0.24          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 1        | 0.24          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 1        | 0.24          |
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 1        | 0.24          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 1        | 0.24          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 8        | 0.24          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 8        | 0.24          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 8        | 0.24          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 8        | 0.24          |
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 8        | 0.24          |
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 8        | 0.24          |
| (1,528) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HB   | 8        | 0.24          |
| (1,373) | 1:109:A:LEU:HD11 | 1:161:A:GLY:HA3  | 6        | 0.24          |
| (1,373) | 1:109:A:LEU:HD12 | 1:161:A:GLY:HA3  | 6        | 0.24          |
| (1,373) | 1:109:A:LEU:HD13 | 1:161:A:GLY:HA3  | 6        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 1        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 1        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 1        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 2        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 2        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 2        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 7        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 7        | 0.24          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 7        | 0.24          |
| (1,347) | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD2  | 5        | 0.24          |
| (1,272) | 1:101:A:VAL:HG21 | 1:120:A:ILE:HD11 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG21 | 1:120:A:ILE:HD12 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG21 | 1:120:A:ILE:HD13 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG22 | 1:120:A:ILE:HD11 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG22 | 1:120:A:ILE:HD12 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG22 | 1:120:A:ILE:HD13 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG23 | 1:120:A:ILE:HD11 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG23 | 1:120:A:ILE:HD12 | 10       | 0.24          |
| (1,272) | 1:101:A:VAL:HG23 | 1:120:A:ILE:HD13 | 10       | 0.24          |
| (1,256) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 4        | 0.24          |
| (1,256) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 4        | 0.24          |
| (1,256) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 4        | 0.24          |
| (1,256) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 5        | 0.24          |
| (1,256) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 5        | 0.24          |
| (1,256) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 5        | 0.24          |
| (1,247) | 1:99:A:LEU:HD21  | 1:140:A:ARG:HG3  | 4        | 0.24          |
| (1,247) | 1:99:A:LEU:HD22  | 1:140:A:ARG:HG3  | 4        | 0.24          |
| (1,247) | 1:99:A:LEU:HD23  | 1:140:A:ARG:HG3  | 4        | 0.24          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 5        | 0.24          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 5        | 0.24          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 5        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 6        | 0.24          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 6        | 0.24          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 6        | 0.24          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG21 | 8        | 0.24          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG22 | 8        | 0.24          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG23 | 8        | 0.24          |
| (1,80)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HD3   | 6        | 0.24          |
| (1,79)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HG3   | 3        | 0.24          |
| (1,51)   | 1:95:A:TRP:HA    | 1:95:A:TRP:HB2   | 10       | 0.24          |
| (1,20)   | 1:93:A:ASP:HB3   | 1:94:A:ARG:HA    | 5        | 0.24          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG21 | 2        | 0.23          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG22 | 2        | 0.23          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG23 | 2        | 0.23          |
| (1,4196) | 1:162:B:THR:H    | 1:102:B:ASN:HB2  | 7        | 0.23          |
| (1,4191) | 1:161:B:GLY:H    | 1:160:B:GLU:HG3  | 1        | 0.23          |
| (1,4052) | 1:151:B:THR:H    | 1:149:B:ASP:HB3  | 1        | 0.23          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG11 | 9        | 0.23          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG12 | 9        | 0.23          |
| (1,4011) | 1:144:B:LEU:H    | 1:148:B:VAL:HG13 | 9        | 0.23          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD11  | 1        | 0.23          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD12  | 1        | 0.23          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD13  | 1        | 0.23          |
| (1,3902) | 1:129:B:ASP:H    | 1:129:B:ASP:HB2  | 9        | 0.23          |
| (1,3893) | 1:128:B:GLN:HE22 | 1:129:B:ASP:H    | 6        | 0.23          |
| (1,3848) | 1:123:B:LYS:H    | 1:109:B:LEU:HG   | 7        | 0.23          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 10       | 0.23          |
| (1,3763) | 1:114:B:LYS:H    | 1:115:B:ASP:HB2  | 5        | 0.23          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 10       | 0.23          |
| (1,3664) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA3  | 3        | 0.23          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD11 | 4        | 0.23          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD12 | 4        | 0.23          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD13 | 4        | 0.23          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD11 | 5        | 0.23          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD12 | 5        | 0.23          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD13 | 5        | 0.23          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 1        | 0.23          |
| (1,3557) | 1:168:B:PRO:HA   | 1:169:B:MET:HG2  | 3        | 0.23          |
| (1,3500) | 1:162:B:THR:HA   | 1:162:B:THR:HG21 | 9        | 0.23          |
| (1,3500) | 1:162:B:THR:HA   | 1:162:B:THR:HG22 | 9        | 0.23          |
| (1,3500) | 1:162:B:THR:HA   | 1:162:B:THR:HG23 | 9        | 0.23          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD21 | 6        | 0.23          |
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD22 | 6        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3499) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HD23 | 6        | 0.23          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 3        | 0.23          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 9        | 0.23          |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 5        | 0.23          |
| (1,3366) | 1:153:B:VAL:HG11 | 1:155:B:SER:HB3  | 5        | 0.23          |
| (1,3366) | 1:153:B:VAL:HG12 | 1:155:B:SER:HB3  | 5        | 0.23          |
| (1,3366) | 1:153:B:VAL:HG13 | 1:155:B:SER:HB3  | 5        | 0.23          |
| (1,3366) | 1:153:B:VAL:HG11 | 1:155:B:SER:HB3  | 6        | 0.23          |
| (1,3366) | 1:153:B:VAL:HG12 | 1:155:B:SER:HB3  | 6        | 0.23          |
| (1,3366) | 1:153:B:VAL:HG13 | 1:155:B:SER:HB3  | 6        | 0.23          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 4        | 0.23          |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 7        | 0.23          |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 7        | 0.23          |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 7        | 0.23          |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 1        | 0.23          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 7        | 0.23          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 7        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 1        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 4        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 6        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 6        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 6        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 6        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 6        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 6        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 6        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 6        | 0.23          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 6        | 0.23          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 4        | 0.23          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 4        | 0.23          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 4        | 0.23          |
| (1,3139) | 1:141:B:LYS:HG3  | 1:141:B:LYS:HE2  | 3        | 0.23          |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 4        | 0.23          |
| (1,3116) | 1:139:B:THR:HG21 | 1:141:B:LYS:HE2  | 2        | 0.23          |
| (1,3116) | 1:139:B:THR:HG22 | 1:141:B:LYS:HE2  | 2        | 0.23          |
| (1,3116) | 1:139:B:THR:HG23 | 1:141:B:LYS:HE2  | 2        | 0.23          |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 10       | 0.23          |
| (1,2982) | 1:125:B:GLU:HA   | 1:126:B:GLU:HG2  | 4        | 0.23          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 3        | 0.23          |
| (1,2930) | 1:120:B:ILE:HG21 | 1:140:B:ARG:HA   | 2        | 0.23          |
| (1,2930) | 1:120:B:ILE:HG22 | 1:140:B:ARG:HA   | 2        | 0.23          |
| (1,2930) | 1:120:B:ILE:HG23 | 1:140:B:ARG:HA   | 2        | 0.23          |
| (1,2929) | 1:120:B:ILE:HG21 | 1:139:B:THR:HA   | 8        | 0.23          |
| (1,2929) | 1:120:B:ILE:HG22 | 1:139:B:THR:HA   | 8        | 0.23          |
| (1,2929) | 1:120:B:ILE:HG23 | 1:139:B:THR:HA   | 8        | 0.23          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 8        | 0.23          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 8        | 0.23          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 8        | 0.23          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 7        | 0.23          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 7        | 0.23          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 7        | 0.23          |
| (1,2776) | 1:113:B:THR:HG21 | 1:116:B:GLY:HA3  | 2        | 0.23          |
| (1,2776) | 1:113:B:THR:HG22 | 1:116:B:GLY:HA3  | 2        | 0.23          |
| (1,2776) | 1:113:B:THR:HG23 | 1:116:B:GLY:HA3  | 2        | 0.23          |
| (1,2749) | 1:112:B:LYS:HG2  | 1:121:B:THR:HB   | 8        | 0.23          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 5        | 0.23          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 5        | 0.23          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 5        | 0.23          |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 6        | 0.23          |
| (1,2627) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HG3  | 3        | 0.23          |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 3        | 0.23          |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 6        | 0.23          |
| (1,2560) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA2  | 10       | 0.23          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD21 | 9        | 0.23          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD22 | 9        | 0.23          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD23 | 9        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 8        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 8        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 8        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 8        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 8        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 8        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 8        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 8        | 0.23          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 8        | 0.23          |
| (1,2484) | 1:99:B:LEU:HA    | 1:100:B:ASP:HB3  | 10       | 0.23          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 5        | 0.23          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 8        | 0.23          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 8        | 0.23          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 8        | 0.23          |
| (1,2352) | 1:95:B:TRP:HB3   | 1:168:B:PRO:HB2  | 8        | 0.23          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 8        | 0.23          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 8        | 0.23          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 8        | 0.23          |
| (1,2332) | 1:95:B:TRP:HA    | 1:95:B:TRP:HB2   | 1        | 0.23          |
| (1,2310) | 1:94:B:ARG:HA    | 1:168:B:PRO:HA   | 7        | 0.23          |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 10       | 0.23          |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 10       | 0.23          |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 10       | 0.23          |
| (1,2215) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 8        | 0.23          |
| (1,2198) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 3        | 0.23          |
| (1,2198) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 3        | 0.23          |
| (1,2198) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 3        | 0.23          |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 10       | 0.23          |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 10       | 0.23          |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 10       | 0.23          |
| (1,2083) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 8        | 0.23          |
| (1,2066) | 1:134:B:ILE:HG21 | 1:138:A:PHE:HB3  | 3        | 0.23          |
| (1,2066) | 1:134:B:ILE:HG22 | 1:138:A:PHE:HB3  | 3        | 0.23          |
| (1,2066) | 1:134:B:ILE:HG23 | 1:138:A:PHE:HB3  | 3        | 0.23          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 1        | 0.23          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 3        | 0.23          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 1        | 0.23          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 5        | 0.23          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 5        | 0.23          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 5        | 0.23          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD21  | 1        | 0.23          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD22  | 1        | 0.23          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD23  | 1        | 0.23          |
| (1,1675) | 1:137:A:CYS:H    | 1:136:A:ARG:HG2  | 4        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1655) | 1:134:A:ILE:H    | 1:127:A:ARG:HG2  | 7        | 0.23          |
| (1,1650) | 1:132:A:GLY:H    | 1:133:A:TYR:HD1  | 4        | 0.23          |
| (1,1650) | 1:132:A:GLY:H    | 1:133:A:TYR:HD2  | 4        | 0.23          |
| (1,1643) | 1:132:A:GLY:H    | 1:130:A:GLU:HB2  | 8        | 0.23          |
| (1,1626) | 1:129:A:ASP:H    | 1:132:A:GLY:HA3  | 2        | 0.23          |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 2        | 0.23          |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 5        | 0.23          |
| (1,1580) | 1:125:A:GLU:H    | 1:108:A:GLU:HG2  | 5        | 0.23          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 10       | 0.23          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 8        | 0.23          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 8        | 0.23          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 8        | 0.23          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 5        | 0.23          |
| (1,1383) | 1:102:A:ASN:HD22 | 1:161:A:GLY:HA3  | 2        | 0.23          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD21 | 4        | 0.23          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD22 | 4        | 0.23          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD23 | 4        | 0.23          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD21 | 7        | 0.23          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD22 | 7        | 0.23          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD23 | 7        | 0.23          |
| (1,1321) | 1:94:A:ARG:H     | 1:93:A:ASP:HA    | 1        | 0.23          |
| (1,1318) | 1:171:A:LYS:HA   | 1:171:A:LYS:HD2  | 5        | 0.23          |
| (1,1314) | 1:170:A:PRO:HB3  | 1:170:A:PRO:HD2  | 7        | 0.23          |
| (1,1289) | 1:169:A:MET:HA   | 1:169:A:MET:HG3  | 8        | 0.23          |
| (1,1193) | 1:158:A:SER:HB3  | 1:160:A:GLU:HB3  | 10       | 0.23          |
| (1,1173) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB3  | 5        | 0.23          |
| (1,1173) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB3  | 5        | 0.23          |
| (1,1173) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB3  | 5        | 0.23          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 2        | 0.23          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 2        | 0.23          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 6        | 0.23          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 2        | 0.23          |
| (1,883)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG21 | 1        | 0.23          |
| (1,883)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG22 | 1        | 0.23          |
| (1,883)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG23 | 1        | 0.23          |
| (1,883)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG21 | 1        | 0.23          |
| (1,883)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG22 | 1        | 0.23          |
| (1,883)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG23 | 1        | 0.23          |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 5        | 0.23          |
| (1,827)  | 1:139:A:THR:HA   | 1:140:A:ARG:HG2  | 2        | 0.23          |
| (1,773)  | 1:130:A:GLU:HA   | 1:130:A:GLU:HG3  | 9        | 0.23          |
| (1,756)  | 1:128:A:GLN:HB3  | 1:133:A:TYR:HD1  | 1        | 0.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,756) | 1:128:A:GLN:HB3  | 1:133:A:TYR:HD2  | 1        | 0.23          |
| (1,747) | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 9        | 0.23          |
| (1,737) | 1:127:A:ARG:HA   | 1:127:A:ARG:HD3  | 2        | 0.23          |
| (1,664) | 1:121:A:THR:HA   | 1:139:A:THR:HA   | 6        | 0.23          |
| (1,648) | 1:120:A:ILE:HG21 | 1:139:A:THR:HA   | 5        | 0.23          |
| (1,648) | 1:120:A:ILE:HG22 | 1:139:A:THR:HA   | 5        | 0.23          |
| (1,648) | 1:120:A:ILE:HG23 | 1:139:A:THR:HA   | 5        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 1        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 4        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 6        | 0.23          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 6        | 0.23          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 10       | 0.23          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 10       | 0.23          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 10       | 0.23          |
| (1,383) | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 3        | 0.23          |
| (1,383) | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 3        | 0.23          |
| (1,383) | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 3        | 0.23          |
| (1,359) | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 1        | 0.23          |
| (1,359) | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 10       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 5        | 0.23          |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 5        | 0.23          |
| (1,358)  | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 5        | 0.23          |
| (1,349)  | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 7        | 0.23          |
| (1,338)  | 1:108:A:GLU:HA   | 1:123:A:LYS:HD2  | 10       | 0.23          |
| (1,336)  | 1:108:A:GLU:HA   | 1:108:A:GLU:HG2  | 8        | 0.23          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 2        | 0.23          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 2        | 0.23          |
| (1,335)  | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 2        | 0.23          |
| (1,280)  | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA3  | 2        | 0.23          |
| (1,255)  | 1:99:A:LEU:HD21  | 1:109:A:LEU:HG   | 9        | 0.23          |
| (1,255)  | 1:99:A:LEU:HD22  | 1:109:A:LEU:HG   | 9        | 0.23          |
| (1,255)  | 1:99:A:LEU:HD23  | 1:109:A:LEU:HG   | 9        | 0.23          |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD11 | 3        | 0.23          |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD12 | 3        | 0.23          |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD13 | 3        | 0.23          |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD21  | 6        | 0.23          |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD22  | 6        | 0.23          |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD23  | 6        | 0.23          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 1        | 0.23          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 1        | 0.23          |
| (1,129)  | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 1        | 0.23          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 6        | 0.23          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 6        | 0.23          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 6        | 0.23          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG21  | 9        | 0.23          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG22  | 9        | 0.23          |
| (1,83)   | 1:96:A:ARG:HA    | 1:97:A:VAL:HG23  | 9        | 0.23          |
| (1,80)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HD2   | 2        | 0.23          |
| (1,72)   | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB3  | 9        | 0.23          |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 6        | 0.23          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG21 | 8        | 0.22          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG22 | 8        | 0.22          |
| (1,4273) | 1:169:B:MET:H    | 1:148:B:VAL:HG23 | 8        | 0.22          |
| (1,4263) | 1:167:B:ALA:H    | 1:166:B:GLU:HB3  | 5        | 0.22          |
| (1,4259) | 1:167:B:ALA:H    | 1:96:B:ARG:HD2   | 3        | 0.22          |
| (1,4192) | 1:161:B:GLY:H    | 1:161:B:GLY:HA2  | 5        | 0.22          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 4        | 0.22          |
| (1,4052) | 1:151:B:THR:H    | 1:149:B:ASP:HB3  | 3        | 0.22          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 1        | 0.22          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 1        | 0.22          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 1        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 2        | 0.22          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 2        | 0.22          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 2        | 0.22          |
| (1,3955) | 1:137:B:CYS:H    | 1:136:B:ARG:HB3  | 1        | 0.22          |
| (1,3955) | 1:137:B:CYS:H    | 1:136:B:ARG:HB3  | 6        | 0.22          |
| (1,3908) | 1:129:B:ASP:H    | 1:132:B:GLY:H    | 8        | 0.22          |
| (1,3861) | 1:125:B:GLU:H    | 1:108:B:GLU:HG2  | 1        | 0.22          |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 5        | 0.22          |
| (1,3795) | 1:118:B:VAL:H    | 1:119:B:GLU:HG3  | 1        | 0.22          |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 1        | 0.22          |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 7        | 0.22          |
| (1,3759) | 1:114:B:LYS:H    | 1:112:B:LYS:HD3  | 8        | 0.22          |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD11 | 9        | 0.22          |
| (1,3680) | 1:107:B:ASP:H    | 1:106:B:PRO:HB2  | 7        | 0.22          |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD11 | 6        | 0.22          |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD12 | 6        | 0.22          |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD13 | 6        | 0.22          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG21 | 2        | 0.22          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG22 | 2        | 0.22          |
| (1,3625) | 1:97:B:VAL:H     | 1:165:B:VAL:HG23 | 2        | 0.22          |
| (1,3604) | 1:94:B:ARG:H     | 1:93:B:ASP:HB3   | 10       | 0.22          |
| (1,3595) | 1:170:B:PRO:HB3  | 1:170:B:PRO:HD2  | 4        | 0.22          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 8        | 0.22          |
| (1,3473) | 1:158:B:SER:HB2  | 1:162:B:THR:HB   | 3        | 0.22          |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 6        | 0.22          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 6        | 0.22          |
| (1,3319) | 1:150:B:PRO:HB2  | 1:150:B:PRO:HD2  | 9        | 0.22          |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 2        | 0.22          |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 10       | 0.22          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 6        | 0.22          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 6        | 0.22          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 6        | 0.22          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 1        | 0.22          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 1        | 0.22          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 1        | 0.22          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 6        | 0.22          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 6        | 0.22          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 6        | 0.22          |
| (1,3139) | 1:141:B:LYS:HG3  | 1:141:B:LYS:HE2  | 4        | 0.22          |
| (1,3137) | 1:141:B:LYS:HG2  | 1:142:B:TYR:HB3  | 4        | 0.22          |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 2        | 0.22          |
| (1,3028) | 1:128:B:GLN:HA   | 1:133:B:TYR:HB2  | 7        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3005) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB3  | 5        | 0.22          |
| (1,2986) | 1:126:B:GLU:HA   | 1:126:B:GLU:HG3  | 8        | 0.22          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 4        | 0.22          |
| (1,2965) | 1:123:B:LYS:HA   | 1:135:B:SER:HB3  | 1        | 0.22          |
| (1,2945) | 1:121:B:THR:HA   | 1:139:B:THR:HA   | 2        | 0.22          |
| (1,2929) | 1:120:B:ILE:HG21 | 1:139:B:THR:HA   | 9        | 0.22          |
| (1,2929) | 1:120:B:ILE:HG22 | 1:139:B:THR:HA   | 9        | 0.22          |
| (1,2929) | 1:120:B:ILE:HG23 | 1:139:B:THR:HA   | 9        | 0.22          |
| (1,2924) | 1:120:B:ILE:HG13 | 1:163:B:LEU:HD11 | 3        | 0.22          |
| (1,2924) | 1:120:B:ILE:HG13 | 1:163:B:LEU:HD12 | 3        | 0.22          |
| (1,2924) | 1:120:B:ILE:HG13 | 1:163:B:LEU:HD13 | 3        | 0.22          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG21 | 4        | 0.22          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG22 | 4        | 0.22          |
| (1,2922) | 1:120:B:ILE:HG13 | 1:120:B:ILE:HG23 | 4        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 5        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 9        | 0.22          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 9        | 0.22          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 5        | 0.22          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 5        | 0.22          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 5        | 0.22          |
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 6        | 0.22          |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 5        | 0.22          |
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 5        | 0.22          |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 5        | 0.22          |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 6        | 0.22          |
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 6        | 0.22          |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 6        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2747) | 1:112:B:LYS:HG3  | 1:119:B:GLU:HA   | 10       | 0.22          |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE3  | 1        | 0.22          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE3  | 8        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG21 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG22 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG23 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG21 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG22 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG23 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG21 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG22 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG23 | 5        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG21 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG22 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG23 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG21 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG22 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG23 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG21 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG22 | 6        | 0.22          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG23 | 6        | 0.22          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 2        | 0.22          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 2        | 0.22          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 2        | 0.22          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 10       | 0.22          |
| (1,2578) | 1:105:B:ALA:HB1  | 1:107:B:ASP:HB3  | 6        | 0.22          |
| (1,2578) | 1:105:B:ALA:HB2  | 1:107:B:ASP:HB3  | 6        | 0.22          |
| (1,2578) | 1:105:B:ALA:HB3  | 1:107:B:ASP:HB3  | 6        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 2        | 0.22          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 2        | 0.22          |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 4        | 0.22          |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 4        | 0.22          |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 4        | 0.22          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD1  | 10       | 0.22          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD2  | 10       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD1  | 10       | 0.22          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD2  | 10       | 0.22          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD1  | 10       | 0.22          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD2  | 10       | 0.22          |
| (1,2282) | 1:88:B:ILE:HG21  | 1:90:B:HIS:HA    | 8        | 0.22          |
| (1,2282) | 1:88:B:ILE:HG22  | 1:90:B:HIS:HA    | 8        | 0.22          |
| (1,2282) | 1:88:B:ILE:HG23  | 1:90:B:HIS:HA    | 8        | 0.22          |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 9        | 0.22          |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 9        | 0.22          |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 9        | 0.22          |
| (1,2169) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 8        | 0.22          |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 9        | 0.22          |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 9        | 0.22          |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 9        | 0.22          |
| (1,2037) | 1:132:A:GLY:HA3  | 1:140:B:ARG:HB3  | 8        | 0.22          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 6        | 0.22          |
| (1,1902) | 1:161:A:GLY:H    | 1:102:A:ASN:HB3  | 3        | 0.22          |
| (1,1844) | 1:154:A:SER:H    | 1:168:A:PRO:HD2  | 7        | 0.22          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 2        | 0.22          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 2        | 0.22          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 2        | 0.22          |
| (1,1703) | 1:142:A:TYR:H    | 1:141:A:LYS:HG3  | 2        | 0.22          |
| (1,1615) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HB3  | 7        | 0.22          |
| (1,1602) | 1:128:A:GLN:H    | 1:128:A:GLN:HB3  | 7        | 0.22          |
| (1,1598) | 1:128:A:GLN:H    | 1:127:A:ARG:HG2  | 1        | 0.22          |
| (1,1581) | 1:125:A:GLU:H    | 1:108:A:GLU:HG3  | 8        | 0.22          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 8        | 0.22          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 9        | 0.22          |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 4        | 0.22          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 1        | 0.22          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 6        | 0.22          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 9        | 0.22          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD11 | 7        | 0.22          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD12 | 7        | 0.22          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD13 | 7        | 0.22          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD22 | 4        | 0.22          |
| (1,1327) | 1:94:A:ARG:H     | 1:169:A:MET:HG2  | 9        | 0.22          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 7        | 0.22          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 7        | 0.22          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 7        | 0.22          |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 8        | 0.22          |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 7        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 7        | 0.22          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 7        | 0.22          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 10       | 0.22          |
| (1,1114) | 1:155:A:SER:HB2  | 1:163:A:LEU:HA   | 8        | 0.22          |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 10       | 0.22          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 9        | 0.22          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 2        | 0.22          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 5        | 0.22          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 8        | 0.22          |
| (1,1014) | 1:148:A:VAL:HG11 | 1:170:A:PRO:HG3  | 9        | 0.22          |
| (1,1014) | 1:148:A:VAL:HG12 | 1:170:A:PRO:HG3  | 9        | 0.22          |
| (1,1014) | 1:148:A:VAL:HG13 | 1:170:A:PRO:HG3  | 9        | 0.22          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 1        | 0.22          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 1        | 0.22          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 1        | 0.22          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 3        | 0.22          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 3        | 0.22          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 3        | 0.22          |
| (1,744)  | 1:127:A:ARG:HB3  | 1:127:A:ARG:HD3  | 4        | 0.22          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 4        | 0.22          |
| (1,717)  | 1:126:A:GLU:HG2  | 1:127:A:ARG:HG3  | 5        | 0.22          |
| (1,700)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG3  | 8        | 0.22          |
| (1,655)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD3  | 6        | 0.22          |
| (1,655)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD3  | 6        | 0.22          |
| (1,655)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD3  | 6        | 0.22          |
| (1,647)  | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 1        | 0.22          |
| (1,647)  | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 1        | 0.22          |
| (1,647)  | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 1        | 0.22          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 2        | 0.22          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 2        | 0.22          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 2        | 0.22          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 2        | 0.22          |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 2        | 0.22          |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 2        | 0.22          |
| (1,558)  | 1:117:A:VAL:HG11 | 1:141:A:LYS:HE2  | 6        | 0.22          |
| (1,558)  | 1:117:A:VAL:HG12 | 1:141:A:LYS:HE2  | 6        | 0.22          |
| (1,558)  | 1:117:A:VAL:HG13 | 1:141:A:LYS:HE2  | 6        | 0.22          |
| (1,521)  | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 5        | 0.22          |
| (1,521)  | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 5        | 0.22          |
| (1,521)  | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 5        | 0.22          |
| (1,502)  | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 3        | 0.22          |
| (1,502)  | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 3        | 0.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,502) | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 3        | 0.22          |
| (1,494) | 1:113:A:THR:HG21 | 1:116:A:GLY:HA2  | 5        | 0.22          |
| (1,494) | 1:113:A:THR:HG22 | 1:116:A:GLY:HA2  | 5        | 0.22          |
| (1,494) | 1:113:A:THR:HG23 | 1:116:A:GLY:HA2  | 5        | 0.22          |
| (1,457) | 1:112:A:LYS:HB2  | 1:120:A:ILE:HA   | 8        | 0.22          |
| (1,457) | 1:112:A:LYS:HB2  | 1:120:A:ILE:HA   | 9        | 0.22          |
| (1,418) | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 8        | 0.22          |
| (1,359) | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 3        | 0.22          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 4        | 0.22          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 4        | 0.22          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 4        | 0.22          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 8        | 0.22          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 8        | 0.22          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 8        | 0.22          |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 2        | 0.22          |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 3        | 0.22          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 7        | 0.22          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 7        | 0.22          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 7        | 0.22          |
| (1,279) | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA2  | 7        | 0.22          |
| (1,256) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HB   | 3        | 0.22          |
| (1,256) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HB   | 3        | 0.22          |
| (1,256) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HB   | 3        | 0.22          |
| (1,229) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG11 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG12 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG13 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG11 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG12 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG13 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG11 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG12 | 9        | 0.22          |
| (1,229) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG13 | 9        | 0.22          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 3        | 0.22          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 3        | 0.22          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 3        | 0.22          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 4        | 0.22          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 4        | 0.22          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 4        | 0.22          |
| (1,108) | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG21  | 2        | 0.22          |
| (1,108) | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG22  | 2        | 0.22          |
| (1,108) | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG23  | 2        | 0.22          |
| (1,72)  | 1:95:A:TRP:HB3   | 1:168:A:PRO:HB3  | 2        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,72)   | 1:95:A:TRP:HB2   | 1:168:A:PRO:HB3  | 3        | 0.22          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG21 | 10       | 0.22          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG22 | 10       | 0.22          |
| (1,68)   | 1:95:A:TRP:HB3   | 1:148:A:VAL:HG23 | 10       | 0.22          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG11 | 6        | 0.22          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG12 | 6        | 0.22          |
| (1,62)   | 1:95:A:TRP:HB2   | 1:148:A:VAL:HG13 | 6        | 0.22          |
| (1,61)   | 1:95:A:TRP:HB2   | 1:96:A:ARG:HA    | 4        | 0.22          |
| (1,4297) | 1:174:B:THR:H    | 1:171:B:LYS:HG3  | 5        | 0.21          |
| (1,4182) | 1:161:B:GLY:H    | 1:102:B:ASN:HB2  | 6        | 0.21          |
| (1,4128) | 1:155:B:SER:H    | 1:154:B:SER:HB2  | 8        | 0.21          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 9        | 0.21          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 9        | 0.21          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 9        | 0.21          |
| (1,4034) | 1:148:B:VAL:H    | 1:149:B:ASP:H    | 5        | 0.21          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 7        | 0.21          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 7        | 0.21          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 7        | 0.21          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD21  | 7        | 0.21          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD22  | 7        | 0.21          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD23  | 7        | 0.21          |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 8        | 0.21          |
| (1,3861) | 1:125:B:GLU:H    | 1:108:B:GLU:HG2  | 2        | 0.21          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 9        | 0.21          |
| (1,3795) | 1:118:B:VAL:H    | 1:119:B:GLU:HG3  | 10       | 0.21          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD21 | 4        | 0.21          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD22 | 4        | 0.21          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD23 | 4        | 0.21          |
| (1,3664) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA3  | 8        | 0.21          |
| (1,3663) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA2  | 5        | 0.21          |
| (1,3654) | 1:102:B:ASN:HD21 | 1:161:B:GLY:HA2  | 3        | 0.21          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG21 | 3        | 0.21          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG22 | 3        | 0.21          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG23 | 3        | 0.21          |
| (1,3599) | 1:171:B:LYS:HA   | 1:171:B:LYS:HD2  | 8        | 0.21          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 9        | 0.21          |
| (1,3481) | 1:159:B:PRO:HA   | 1:159:B:PRO:HG3  | 7        | 0.21          |
| (1,3458) | 1:157:B:LEU:HD21 | 1:161:B:GLY:HA3  | 8        | 0.21          |
| (1,3458) | 1:157:B:LEU:HD22 | 1:161:B:GLY:HA3  | 8        | 0.21          |
| (1,3458) | 1:157:B:LEU:HD23 | 1:161:B:GLY:HA3  | 8        | 0.21          |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 10       | 0.21          |
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 10       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 10       | 0.21          |
| (1,3430) | 1:157:B:LEU:HA   | 1:163:B:LEU:HB3  | 9        | 0.21          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 8        | 0.21          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD21 | 1        | 0.21          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD22 | 1        | 0.21          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD23 | 1        | 0.21          |
| (1,3409) | 1:155:B:SER:HB2  | 1:157:B:LEU:HB3  | 9        | 0.21          |
| (1,3358) | 1:153:B:VAL:HA   | 1:168:B:PRO:HD2  | 10       | 0.21          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG21 | 3        | 0.21          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG22 | 3        | 0.21          |
| (1,3327) | 1:150:B:PRO:HD2  | 1:151:B:THR:HG23 | 3        | 0.21          |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 5        | 0.21          |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 7        | 0.21          |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 2        | 0.21          |
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 2        | 0.21          |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 2        | 0.21          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 6        | 0.21          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 6        | 0.21          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 6        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 2        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 5        | 0.21          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 5        | 0.21          |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 7        | 0.21          |
| (1,3108) | 1:139:B:THR:HA   | 1:140:B:ARG:HG2  | 9        | 0.21          |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 7        | 0.21          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE1  | 2        | 0.21          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE2  | 2        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3015) | 1:127:B:ARG:HA   | 1:127:B:ARG:HB3  | 7        | 0.21          |
| (1,3010) | 1:126:B:GLU:HG3  | 1:133:B:TYR:HB3  | 7        | 0.21          |
| (1,2999) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HB3  | 1        | 0.21          |
| (1,2984) | 1:125:B:GLU:HA   | 1:135:B:SER:HB2  | 1        | 0.21          |
| (1,2981) | 1:125:B:GLU:HA   | 1:125:B:GLU:HG3  | 2        | 0.21          |
| (1,2973) | 1:123:B:LYS:HG3  | 1:137:B:CYS:HB2  | 10       | 0.21          |
| (1,2945) | 1:121:B:THR:HA   | 1:139:B:THR:HA   | 3        | 0.21          |
| (1,2928) | 1:120:B:ILE:HG21 | 1:122:B:GLY:HA3  | 9        | 0.21          |
| (1,2928) | 1:120:B:ILE:HG22 | 1:122:B:GLY:HA3  | 9        | 0.21          |
| (1,2928) | 1:120:B:ILE:HG23 | 1:122:B:GLY:HA3  | 9        | 0.21          |
| (1,2894) | 1:119:B:GLU:HB3  | 1:121:B:THR:HB   | 9        | 0.21          |
| (1,2894) | 1:119:B:GLU:HB3  | 1:121:B:THR:HB   | 10       | 0.21          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 3        | 0.21          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 3        | 0.21          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 3        | 0.21          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG21 | 9        | 0.21          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG22 | 9        | 0.21          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG23 | 9        | 0.21          |
| (1,2738) | 1:112:B:LYS:HB2  | 1:120:B:ILE:HA   | 9        | 0.21          |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE3  | 2        | 0.21          |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE3  | 2        | 0.21          |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE3  | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 2        | 0.21          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 2        | 0.21          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 4        | 0.21          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 4        | 0.21          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 4        | 0.21          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 8        | 0.21          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 8        | 0.21          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 8        | 0.21          |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 2        | 0.21          |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 8        | 0.21          |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 10       | 0.21          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 8        | 0.21          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 8        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 8        | 0.21          |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 2        | 0.21          |
| (1,2560) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA2  | 8        | 0.21          |
| (1,2559) | 1:102:B:ASN:HB2  | 1:161:B:GLY:HA3  | 5        | 0.21          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD21 | 3        | 0.21          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD22 | 3        | 0.21          |
| (1,2558) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD23 | 3        | 0.21          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD11 | 8        | 0.21          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD12 | 8        | 0.21          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD13 | 8        | 0.21          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 6        | 0.21          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 8        | 0.21          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 9        | 0.21          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 6        | 0.21          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 6        | 0.21          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 6        | 0.21          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG21  | 2        | 0.21          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG22  | 2        | 0.21          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG23  | 2        | 0.21          |
| (1,2341) | 1:95:B:TRP:HB2   | 1:95:B:TRP:HE3   | 10       | 0.21          |
| (1,2306) | 1:94:B:ARG:HA    | 1:94:B:ARG:HG3   | 7        | 0.21          |
| (1,2215) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 1        | 0.21          |
| (1,2212) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 3        | 0.21          |
| (1,2150) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB3  | 6        | 0.21          |
| (1,2150) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB3  | 6        | 0.21          |
| (1,2150) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB3  | 6        | 0.21          |
| (1,2083) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 1        | 0.21          |
| (1,2080) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD2  | 3        | 0.21          |
| (1,2018) | 1:97:B:VAL:HG11  | 1:131:A:HIS:HB3  | 6        | 0.21          |
| (1,2018) | 1:97:B:VAL:HG12  | 1:131:A:HIS:HB3  | 6        | 0.21          |
| (1,2018) | 1:97:B:VAL:HG13  | 1:131:A:HIS:HB3  | 6        | 0.21          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 2        | 0.21          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG11 | 2        | 0.21          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG12 | 2        | 0.21          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG13 | 2        | 0.21          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG21 | 1        | 0.21          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG22 | 1        | 0.21          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG23 | 1        | 0.21          |
| (1,1816) | 1:153:A:VAL:H    | 1:149:A:ASP:HB2  | 2        | 0.21          |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 1        | 0.21          |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 4        | 0.21          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 3        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 3        | 0.21          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 3        | 0.21          |
| (1,1653) | 1:132:A:GLY:H    | 1:134:A:ILE:HG21 | 6        | 0.21          |
| (1,1653) | 1:132:A:GLY:H    | 1:134:A:ILE:HG22 | 6        | 0.21          |
| (1,1653) | 1:132:A:GLY:H    | 1:134:A:ILE:HG23 | 6        | 0.21          |
| (1,1647) | 1:132:A:GLY:H    | 1:131:A:HIS:HB3  | 6        | 0.21          |
| (1,1647) | 1:132:A:GLY:H    | 1:131:A:HIS:HB3  | 9        | 0.21          |
| (1,1626) | 1:129:A:ASP:H    | 1:132:A:GLY:HA3  | 8        | 0.21          |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 4        | 0.21          |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 3        | 0.21          |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 4        | 0.21          |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 8        | 0.21          |
| (1,1611) | 1:128:A:GLN:HE22 | 1:128:A:GLN:H    | 6        | 0.21          |
| (1,1580) | 1:125:A:GLU:H    | 1:108:A:GLU:HG2  | 1        | 0.21          |
| (1,1545) | 1:120:A:ILE:H    | 1:140:A:ARG:HG3  | 9        | 0.21          |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD11 | 5        | 0.21          |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD12 | 5        | 0.21          |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD13 | 5        | 0.21          |
| (1,1517) | 1:118:A:VAL:H    | 1:142:A:TYR:HB2  | 6        | 0.21          |
| (1,1514) | 1:118:A:VAL:H    | 1:119:A:GLU:HG3  | 5        | 0.21          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 2        | 0.21          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 3        | 0.21          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 4        | 0.21          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 7        | 0.21          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD21 | 2        | 0.21          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD22 | 2        | 0.21          |
| (1,1381) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD23 | 2        | 0.21          |
| (1,1369) | 1:102:A:ASN:HD21 | 1:109:A:LEU:HD11 | 3        | 0.21          |
| (1,1369) | 1:102:A:ASN:HD21 | 1:109:A:LEU:HD12 | 3        | 0.21          |
| (1,1369) | 1:102:A:ASN:HD21 | 1:109:A:LEU:HD13 | 3        | 0.21          |
| (1,1326) | 1:94:A:ARG:H     | 1:168:A:PRO:HA   | 5        | 0.21          |
| (1,1314) | 1:170:A:PRO:HB3  | 1:170:A:PRO:HD3  | 9        | 0.21          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 1        | 0.21          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 1        | 0.21          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 1        | 0.21          |
| (1,1210) | 1:160:A:GLU:HB2  | 1:162:A:THR:HB   | 8        | 0.21          |
| (1,1193) | 1:158:A:SER:HB3  | 1:160:A:GLU:HB3  | 3        | 0.21          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 4        | 0.21          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 7        | 0.21          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 9        | 0.21          |
| (1,1038) | 1:150:A:PRO:HB2  | 1:150:A:PRO:HD2  | 7        | 0.21          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 1        | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,962) | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 9        | 0.21          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 7        | 0.21          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 7        | 0.21          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 7        | 0.21          |
| (1,842) | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 4        | 0.21          |
| (1,842) | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 8        | 0.21          |
| (1,842) | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 9        | 0.21          |
| (1,827) | 1:139:A:THR:HA   | 1:140:A:ARG:HG2  | 7        | 0.21          |
| (1,737) | 1:127:A:ARG:HA   | 1:127:A:ARG:HD3  | 6        | 0.21          |
| (1,736) | 1:127:A:ARG:HA   | 1:127:A:ARG:HG3  | 7        | 0.21          |
| (1,710) | 1:126:A:GLU:HA   | 1:135:A:SER:HB2  | 6        | 0.21          |
| (1,647) | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 5        | 0.21          |
| (1,647) | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 5        | 0.21          |
| (1,647) | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 5        | 0.21          |
| (1,641) | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG21 | 3        | 0.21          |
| (1,641) | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG22 | 3        | 0.21          |
| (1,641) | 1:120:A:ILE:HG13 | 1:120:A:ILE:HG23 | 3        | 0.21          |
| (1,612) | 1:119:A:GLU:HA   | 1:141:A:LYS:HE3  | 6        | 0.21          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD21 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD22 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG11 | 1:144:A:LEU:HD23 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD21 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD22 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG12 | 1:144:A:LEU:HD23 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD21 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD22 | 9        | 0.21          |
| (1,588) | 1:118:A:VAL:HG13 | 1:144:A:LEU:HD23 | 9        | 0.21          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 9        | 0.21          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 9        | 0.21          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 9        | 0.21          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 9        | 0.21          |
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 9        | 0.21          |
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 9        | 0.21          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 3        | 0.21          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 3        | 0.21          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 3        | 0.21          |
| (1,473) | 1:112:A:LYS:HE2  | 1:114:A:LYS:HB2  | 8        | 0.21          |
| (1,472) | 1:112:A:LYS:HD2  | 1:120:A:ILE:HA   | 3        | 0.21          |
| (1,453) | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 1        | 0.21          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG21 | 7        | 0.21          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG22 | 7        | 0.21          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG23 | 7        | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG21 | 7        | 0.21          |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG22 | 7        | 0.21          |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG23 | 7        | 0.21          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG21 | 7        | 0.21          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG22 | 7        | 0.21          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG23 | 7        | 0.21          |
| (1,404) | 1:110:A:THR:HG21 | 1:112:A:LYS:HB2  | 9        | 0.21          |
| (1,404) | 1:110:A:THR:HG22 | 1:112:A:LYS:HB2  | 9        | 0.21          |
| (1,404) | 1:110:A:THR:HG23 | 1:112:A:LYS:HB2  | 9        | 0.21          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD11 | 5        | 0.21          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD12 | 5        | 0.21          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD13 | 5        | 0.21          |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 5        | 0.21          |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 9        | 0.21          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 3        | 0.21          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 3        | 0.21          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 3        | 0.21          |
| (1,306) | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 3        | 0.21          |
| (1,306) | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 10       | 0.21          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 1        | 0.21          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 2        | 0.21          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 6        | 0.21          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 8        | 0.21          |
| (1,279) | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA2  | 9        | 0.21          |
| (1,248) | 1:99:A:LEU:HD21  | 1:140:A:ARG:HD2  | 6        | 0.21          |
| (1,248) | 1:99:A:LEU:HD22  | 1:140:A:ARG:HD2  | 6        | 0.21          |
| (1,248) | 1:99:A:LEU:HD23  | 1:140:A:ARG:HD2  | 6        | 0.21          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 4        | 0.21          |
| (1,240) | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 4        | 0.21          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD11 | 5        | 0.21          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD12 | 5        | 0.21          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD13 | 5        | 0.21          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG11 | 10       | 0.21          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG12 | 10       | 0.21          |
| (1,129) | 1:97:A:VAL:HB    | 1:148:A:VAL:HG13 | 10       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4205) | 1:162:B:THR:H    | 1:160:B:GLU:HB2  | 8        | 0.2           |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG21 | 1        | 0.2           |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG22 | 1        | 0.2           |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG23 | 1        | 0.2           |
| (1,4183) | 1:161:B:GLY:H    | 1:102:B:ASN:HB3  | 8        | 0.2           |
| (1,4182) | 1:161:B:GLY:H    | 1:102:B:ASN:HB2  | 2        | 0.2           |
| (1,4141) | 1:156:B:SER:H    | 1:157:B:LEU:HB3  | 3        | 0.2           |
| (1,4115) | 1:154:B:SER:H    | 1:155:B:SER:HB2  | 5        | 0.2           |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 4        | 0.2           |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 4        | 0.2           |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 4        | 0.2           |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD11  | 5        | 0.2           |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD12  | 5        | 0.2           |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD13  | 5        | 0.2           |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 7        | 0.2           |
| (1,3868) | 1:126:B:GLU:H    | 1:125:B:GLU:HG2  | 4        | 0.2           |
| (1,3847) | 1:123:B:LYS:H    | 1:109:B:LEU:HB2  | 8        | 0.2           |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 6        | 0.2           |
| (1,3806) | 1:119:B:GLU:H    | 1:114:B:LYS:HB3  | 7        | 0.2           |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 7        | 0.2           |
| (1,3795) | 1:118:B:VAL:H    | 1:119:B:GLU:HG3  | 8        | 0.2           |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 8        | 0.2           |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 10       | 0.2           |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 2        | 0.2           |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 10       | 0.2           |
| (1,3358) | 1:153:B:VAL:HA   | 1:168:B:PRO:HD2  | 3        | 0.2           |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 6        | 0.2           |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 8        | 0.2           |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG2  | 9        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 3        | 0.2           |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 3        | 0.2           |
| (1,3133) | 1:141:B:LYS:HG2  | 1:141:B:LYS:HE2  | 5        | 0.2           |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 1        | 0.2           |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 8        | 0.2           |
| (1,3093) | 1:136:B:ARG:HA   | 1:136:B:ARG:HD2  | 8        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD11 | 8        | 0.2           |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD12 | 8        | 0.2           |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD13 | 8        | 0.2           |
| (1,3018) | 1:127:B:ARG:HA   | 1:127:B:ARG:HD3  | 3        | 0.2           |
| (1,2981) | 1:125:B:GLU:HA   | 1:125:B:GLU:HG3  | 1        | 0.2           |
| (1,2891) | 1:119:B:GLU:HA   | 1:141:B:LYS:HD3  | 10       | 0.2           |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 7        | 0.2           |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 7        | 0.2           |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 7        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 4        | 0.2           |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 4        | 0.2           |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 5        | 0.2           |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 7        | 0.2           |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 8        | 0.2           |
| (1,2628) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HD2  | 9        | 0.2           |
| (1,2626) | 1:108:B:GLU:HG2  | 1:123:B:LYS:HE2  | 1        | 0.2           |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 1        | 0.2           |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 2        | 0.2           |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 5        | 0.2           |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 6        | 0.2           |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 7        | 0.2           |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 9        | 0.2           |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 9        | 0.2           |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 2        | 0.2           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 6        | 0.2           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 6        | 0.2           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 6        | 0.2           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 8        | 0.2           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 8        | 0.2           |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 8        | 0.2           |
| (1,2540) | 1:100:B:ASP:HA   | 1:100:B:ASP:HB3  | 4        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 6        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 6        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 6        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 6        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 6        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 6        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 6        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 6        | 0.2           |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 6        | 0.2           |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD11 | 3        | 0.2           |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD12 | 3        | 0.2           |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD13 | 3        | 0.2           |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 1        | 0.2           |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 1        | 0.2           |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 1        | 0.2           |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 5        | 0.2           |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 3        | 0.2           |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 3        | 0.2           |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 3        | 0.2           |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 8        | 0.2           |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 8        | 0.2           |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 8        | 0.2           |
| (1,2297) | 1:93:B:ASP:HA    | 1:94:B:ARG:HD2   | 6        | 0.2           |
| (1,2281) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 7        | 0.2           |
| (1,2148) | 1:143:A:THR:H    | 1:132:B:GLY:HA2  | 7        | 0.2           |
| (1,2006) | 1:171:A:LYS:H    | 1:170:A:PRO:HG3  | 5        | 0.2           |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD11 | 10       | 0.2           |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD12 | 10       | 0.2           |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD13 | 10       | 0.2           |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG21 | 3        | 0.2           |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG22 | 3        | 0.2           |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG23 | 3        | 0.2           |
| (1,1796) | 1:152:A:GLN:HE21 | 1:149:A:ASP:HB2  | 2        | 0.2           |
| (1,1733) | 1:147:A:GLY:H    | 1:146:A:PRO:HG2  | 3        | 0.2           |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 6        | 0.2           |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 6        | 0.2           |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 6        | 0.2           |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD11  | 5        | 0.2           |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD12  | 5        | 0.2           |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD13  | 5        | 0.2           |
| (1,1664) | 1:135:A:SER:H    | 1:134:A:ILE:HG13 | 8        | 0.2           |
| (1,1621) | 1:129:A:ASP:H    | 1:129:A:ASP:HB2  | 10       | 0.2           |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 2        | 0.2           |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD1  | 9        | 0.2           |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD2  | 9        | 0.2           |
| (1,1576) | 1:124:A:HIS:H    | 1:136:A:ARG:HA   | 3        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 10       | 0.2           |
| (1,1545) | 1:120:A:ILE:H    | 1:140:A:ARG:HG3  | 5        | 0.2           |
| (1,1489) | 1:114:A:LYS:H    | 1:119:A:GLU:H    | 6        | 0.2           |
| (1,1391) | 1:105:A:ALA:H    | 1:108:A:GLU:HB3  | 4        | 0.2           |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD22 | 2        | 0.2           |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG21 | 4        | 0.2           |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG22 | 4        | 0.2           |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG23 | 4        | 0.2           |
| (1,1314) | 1:170:A:PRO:HB3  | 1:170:A:PRO:HD2  | 2        | 0.2           |
| (1,1210) | 1:160:A:GLU:HB2  | 1:162:A:THR:HB   | 1        | 0.2           |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 9        | 0.2           |
| (1,1173) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB3  | 1        | 0.2           |
| (1,1173) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB3  | 1        | 0.2           |
| (1,1173) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB3  | 1        | 0.2           |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 1        | 0.2           |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 4        | 0.2           |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD21 | 6        | 0.2           |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD22 | 6        | 0.2           |
| (1,1140) | 1:156:A:SER:HB3  | 1:157:A:LEU:HD23 | 6        | 0.2           |
| (1,1077) | 1:153:A:VAL:HA   | 1:168:A:PRO:HD2  | 4        | 0.2           |
| (1,1014) | 1:148:A:VAL:HG11 | 1:170:A:PRO:HG3  | 7        | 0.2           |
| (1,1014) | 1:148:A:VAL:HG12 | 1:170:A:PRO:HG3  | 7        | 0.2           |
| (1,1014) | 1:148:A:VAL:HG13 | 1:170:A:PRO:HG3  | 7        | 0.2           |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 4        | 0.2           |
| (1,967)  | 1:146:A:PRO:HB3  | 1:147:A:GLY:HA2  | 10       | 0.2           |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 6        | 0.2           |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 6        | 0.2           |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 6        | 0.2           |
| (1,858)  | 1:141:A:LYS:HG3  | 1:141:A:LYS:HE2  | 2        | 0.2           |
| (1,857)  | 1:141:A:LYS:HG2  | 1:143:A:THR:HA   | 8        | 0.2           |
| (1,849)  | 1:141:A:LYS:HB2  | 1:141:A:LYS:HE2  | 1        | 0.2           |
| (1,842)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 3        | 0.2           |
| (1,815)  | 1:136:A:ARG:HG3  | 1:138:A:PHE:HA   | 6        | 0.2           |
| (1,773)  | 1:130:A:GLU:HA   | 1:130:A:GLU:HG3  | 7        | 0.2           |
| (1,749)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HE1  | 6        | 0.2           |
| (1,749)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HE2  | 6        | 0.2           |
| (1,746)  | 1:128:A:GLN:HA   | 1:128:A:GLN:HG3  | 9        | 0.2           |
| (1,746)  | 1:128:A:GLN:HA   | 1:128:A:GLN:HG3  | 10       | 0.2           |
| (1,705)  | 1:126:A:GLU:HA   | 1:126:A:GLU:HG3  | 10       | 0.2           |
| (1,700)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG3  | 6        | 0.2           |
| (1,647)  | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 2        | 0.2           |
| (1,647)  | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 2        | 0.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,647) | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 2        | 0.2           |
| (1,643) | 1:120:A:ILE:HG13 | 1:163:A:LEU:HD11 | 2        | 0.2           |
| (1,643) | 1:120:A:ILE:HG13 | 1:163:A:LEU:HD12 | 2        | 0.2           |
| (1,643) | 1:120:A:ILE:HG13 | 1:163:A:LEU:HD13 | 2        | 0.2           |
| (1,635) | 1:120:A:ILE:HB   | 1:140:A:ARG:HD2  | 8        | 0.2           |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 3        | 0.2           |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 3        | 0.2           |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 3        | 0.2           |
| (1,514) | 1:115:A:ASP:HB2  | 1:143:A:THR:HG21 | 10       | 0.2           |
| (1,514) | 1:115:A:ASP:HB2  | 1:143:A:THR:HG22 | 10       | 0.2           |
| (1,514) | 1:115:A:ASP:HB2  | 1:143:A:THR:HG23 | 10       | 0.2           |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG21 | 6        | 0.2           |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG22 | 6        | 0.2           |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG23 | 6        | 0.2           |
| (1,489) | 1:113:A:THR:HB   | 1:150:A:PRO:HB2  | 4        | 0.2           |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 6        | 0.2           |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 9        | 0.2           |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 9        | 0.2           |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 3        | 0.2           |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 3        | 0.2           |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 3        | 0.2           |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 6        | 0.2           |
| (1,306) | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 1        | 0.2           |
| (1,306) | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 2        | 0.2           |
| (1,306) | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 4        | 0.2           |
| (1,306) | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 5        | 0.2           |
| (1,306) | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 6        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,306)  | 1:106:A:PRO:HA   | 1:106:A:PRO:HB3  | 9        | 0.2           |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 9        | 0.2           |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 9        | 0.2           |
| (1,269)  | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 9        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 6        | 0.2           |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 6        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG11 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG12 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG13 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG11 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG12 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG13 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG11 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG12 | 1        | 0.2           |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG13 | 1        | 0.2           |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD11 | 1        | 0.2           |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD12 | 1        | 0.2           |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD13 | 1        | 0.2           |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD11 | 8        | 0.2           |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD12 | 8        | 0.2           |
| (1,216)  | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD13 | 8        | 0.2           |
| (1,175)  | 1:98:A:SER:HA    | 1:142:A:TYR:HE1  | 3        | 0.2           |
| (1,175)  | 1:98:A:SER:HA    | 1:142:A:TYR:HE2  | 3        | 0.2           |
| (1,102)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HB3  | 10       | 0.2           |
| (1,96)   | 1:96:A:ARG:HB2   | 1:166:A:GLU:HB2  | 8        | 0.2           |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG21 | 9        | 0.2           |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG22 | 9        | 0.2           |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG23 | 9        | 0.2           |
| (1,23)   | 1:94:A:ARG:HA    | 1:94:A:ARG:HB3   | 6        | 0.2           |
| (1,4281) | 1:169:B:MET:H    | 1:169:B:MET:HG3  | 5        | 0.19          |
| (1,4263) | 1:167:B:ALA:H    | 1:166:B:GLU:HB3  | 4        | 0.19          |
| (1,4089) | 1:152:B:GLN:HE22 | 1:152:B:GLN:HB2  | 1        | 0.19          |
| (1,4089) | 1:152:B:GLN:HE22 | 1:152:B:GLN:HB2  | 2        | 0.19          |
| (1,4084) | 1:152:B:GLN:HE21 | 1:168:B:PRO:HD2  | 5        | 0.19          |
| (1,4082) | 1:152:B:GLN:HE21 | 1:167:B:ALA:HB1  | 3        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4082) | 1:152:B:GLN:HE21 | 1:167:B:ALA:HB2  | 3        | 0.19          |
| (1,4082) | 1:152:B:GLN:HE21 | 1:167:B:ALA:HB3  | 3        | 0.19          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 8        | 0.19          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 8        | 0.19          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 8        | 0.19          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD11  | 10       | 0.19          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD12  | 10       | 0.19          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD13  | 10       | 0.19          |
| (1,3915) | 1:131:B:HIS:H    | 1:129:B:ASP:HB3  | 8        | 0.19          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD11 | 1        | 0.19          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD12 | 1        | 0.19          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD13 | 1        | 0.19          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD11 | 10       | 0.19          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD12 | 10       | 0.19          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD13 | 10       | 0.19          |
| (1,3806) | 1:119:B:GLU:H    | 1:114:B:LYS:HB3  | 1        | 0.19          |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 4        | 0.19          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 8        | 0.19          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 8        | 0.19          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 8        | 0.19          |
| (1,3726) | 1:111:B:VAL:H    | 1:110:B:THR:HB   | 8        | 0.19          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD21 | 8        | 0.19          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD22 | 8        | 0.19          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD23 | 8        | 0.19          |
| (1,3607) | 1:94:B:ARG:H     | 1:168:B:PRO:HA   | 3        | 0.19          |
| (1,3607) | 1:94:B:ARG:H     | 1:168:B:PRO:HA   | 4        | 0.19          |
| (1,3595) | 1:170:B:PRO:HB3  | 1:170:B:PRO:HD2  | 6        | 0.19          |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 1        | 0.19          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 10       | 0.19          |
| (1,3470) | 1:158:B:SER:HA   | 1:160:B:GLU:HB3  | 9        | 0.19          |
| (1,3454) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB3  | 1        | 0.19          |
| (1,3454) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB3  | 1        | 0.19          |
| (1,3454) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB3  | 1        | 0.19          |
| (1,3430) | 1:157:B:LEU:HA   | 1:163:B:LEU:HB3  | 4        | 0.19          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 4        | 0.19          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 5        | 0.19          |
| (1,3424) | 1:157:B:LEU:HA   | 1:157:B:LEU:HB2  | 7        | 0.19          |
| (1,3391) | 1:155:B:SER:HA   | 1:165:B:VAL:HA   | 9        | 0.19          |
| (1,3358) | 1:153:B:VAL:HA   | 1:168:B:PRO:HD2  | 1        | 0.19          |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 4        | 0.19          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 2        | 0.19          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 2        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 2        | 0.19          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 2        | 0.19          |
| (1,3143) | 1:141:B:LYS:HG3  | 1:142:B:TYR:HB3  | 6        | 0.19          |
| (1,3143) | 1:141:B:LYS:HG3  | 1:142:B:TYR:HB3  | 7        | 0.19          |
| (1,3138) | 1:141:B:LYS:HG2  | 1:143:B:THR:HA   | 10       | 0.19          |
| (1,3120) | 1:140:B:ARG:HB2  | 1:140:B:ARG:HD2  | 3        | 0.19          |
| (1,2971) | 1:123:B:LYS:HB3  | 1:137:B:CYS:HB2  | 3        | 0.19          |
| (1,2969) | 1:123:B:LYS:HB2  | 1:137:B:CYS:HB3  | 3        | 0.19          |
| (1,2928) | 1:120:B:ILE:HG21 | 1:122:B:GLY:HA3  | 8        | 0.19          |
| (1,2928) | 1:120:B:ILE:HG22 | 1:122:B:GLY:HA3  | 8        | 0.19          |
| (1,2928) | 1:120:B:ILE:HG23 | 1:122:B:GLY:HA3  | 8        | 0.19          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD11 | 3        | 0.19          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD12 | 3        | 0.19          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD13 | 3        | 0.19          |
| (1,2892) | 1:119:B:GLU:HA   | 1:141:B:LYS:HE2  | 10       | 0.19          |
| (1,2870) | 1:118:B:VAL:HG11 | 1:148:B:VAL:HB   | 2        | 0.19          |
| (1,2870) | 1:118:B:VAL:HG12 | 1:148:B:VAL:HB   | 2        | 0.19          |
| (1,2870) | 1:118:B:VAL:HG13 | 1:148:B:VAL:HB   | 2        | 0.19          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 9        | 0.19          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 9        | 0.19          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 9        | 0.19          |
| (1,2759) | 1:112:B:LYS:HE3  | 1:121:B:THR:HB   | 4        | 0.19          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE3  | 9        | 0.19          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 1        | 0.19          |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 9        | 0.19          |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 10       | 0.19          |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 10       | 0.19          |
| (1,2560) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA2  | 6        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG11 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG12 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG13 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG11 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG12 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG13 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG11 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG12 | 4        | 0.19          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG13 | 4        | 0.19          |
| (1,2518) | 1:99:B:LEU:HD21  | 1:101:B:VAL:HB   | 4        | 0.19          |
| (1,2518) | 1:99:B:LEU:HD22  | 1:101:B:VAL:HB   | 4        | 0.19          |
| (1,2518) | 1:99:B:LEU:HD23  | 1:101:B:VAL:HB   | 4        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 5        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 5        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 5        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 5        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 5        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 5        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 5        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 5        | 0.19          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 5        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG21 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG22 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG23 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG21 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG22 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG23 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG21 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG22 | 4        | 0.19          |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG23 | 4        | 0.19          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD11 | 9        | 0.19          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD12 | 9        | 0.19          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD13 | 9        | 0.19          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG21  | 6        | 0.19          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG22  | 6        | 0.19          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG23  | 6        | 0.19          |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 7        | 0.19          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 10       | 0.19          |
| (1,2329) | 1:94:B:ARG:HD2   | 1:168:B:PRO:HA   | 10       | 0.19          |
| (1,2215) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 2        | 0.19          |
| (1,2209) | 1:134:A:ILE:HA   | 1:140:B:ARG:HB3  | 4        | 0.19          |
| (1,2205) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HD2  | 2        | 0.19          |
| (1,2205) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HD2  | 2        | 0.19          |
| (1,2205) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HD2  | 2        | 0.19          |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 1        | 0.19          |
| (1,2083) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 2        | 0.19          |
| (1,2077) | 1:134:A:ILE:HA   | 1:140:B:ARG:HB3  | 4        | 0.19          |
| (1,2073) | 1:134:B:ILE:HD11 | 1:140:A:ARG:HD2  | 2        | 0.19          |
| (1,2073) | 1:134:B:ILE:HD12 | 1:140:A:ARG:HD2  | 2        | 0.19          |
| (1,2073) | 1:134:B:ILE:HD13 | 1:140:A:ARG:HD2  | 2        | 0.19          |
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 1        | 0.19          |
| (1,1958) | 1:165:A:VAL:H    | 1:166:A:GLU:HB3  | 5        | 0.19          |
| (1,1925) | 1:162:A:THR:H    | 1:160:A:GLU:HG2  | 6        | 0.19          |
| (1,1924) | 1:162:A:THR:H    | 1:160:A:GLU:HB2  | 7        | 0.19          |
| (1,1913) | 1:161:A:GLY:H    | 1:162:A:THR:HB   | 2        | 0.19          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 8        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1902) | 1:161:A:GLY:H    | 1:102:A:ASN:HB3  | 4        | 0.19          |
| (1,1901) | 1:161:A:GLY:H    | 1:102:A:ASN:HB2  | 7        | 0.19          |
| (1,1860) | 1:156:A:SER:H    | 1:157:A:LEU:HB3  | 6        | 0.19          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 4        | 0.19          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 4        | 0.19          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 4        | 0.19          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG21 | 10       | 0.19          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG22 | 10       | 0.19          |
| (1,1797) | 1:152:A:GLN:HE21 | 1:151:A:THR:HG23 | 10       | 0.19          |
| (1,1767) | 1:149:A:ASP:H    | 1:170:A:PRO:HG3  | 2        | 0.19          |
| (1,1738) | 1:148:A:VAL:H    | 1:144:A:LEU:HB2  | 6        | 0.19          |
| (1,1657) | 1:134:A:ILE:H    | 1:133:A:TYR:HB3  | 6        | 0.19          |
| (1,1647) | 1:132:A:GLY:H    | 1:131:A:HIS:HB3  | 10       | 0.19          |
| (1,1634) | 1:131:A:HIS:H    | 1:129:A:ASP:HB3  | 10       | 0.19          |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 9        | 0.19          |
| (1,1608) | 1:128:A:GLN:HE22 | 1:128:A:GLN:HB2  | 3        | 0.19          |
| (1,1584) | 1:125:A:GLU:H    | 1:126:A:GLU:H    | 9        | 0.19          |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 7        | 0.19          |
| (1,1514) | 1:118:A:VAL:H    | 1:119:A:GLU:HG3  | 6        | 0.19          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 1        | 0.19          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 1        | 0.19          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 1        | 0.19          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 5        | 0.19          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 5        | 0.19          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 5        | 0.19          |
| (1,1408) | 1:107:A:ASP:H    | 1:109:A:LEU:HD11 | 1        | 0.19          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD21 | 8        | 0.19          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD22 | 8        | 0.19          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD23 | 8        | 0.19          |
| (1,1383) | 1:102:A:ASN:HD22 | 1:161:A:GLY:HA3  | 4        | 0.19          |
| (1,1373) | 1:102:A:ASN:HD21 | 1:161:A:GLY:HA2  | 7        | 0.19          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD11 | 4        | 0.19          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD12 | 4        | 0.19          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD13 | 4        | 0.19          |
| (1,1367) | 1:102:A:ASN:H    | 1:102:A:ASN:HD22 | 7        | 0.19          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 1        | 0.19          |
| (1,1282) | 1:168:A:PRO:HB3  | 1:169:A:MET:HA   | 2        | 0.19          |
| (1,1282) | 1:168:A:PRO:HB3  | 1:169:A:MET:HA   | 4        | 0.19          |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 4        | 0.19          |
| (1,1173) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB3  | 3        | 0.19          |
| (1,1173) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB3  | 3        | 0.19          |
| (1,1173) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB3  | 3        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1173) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB3  | 6        | 0.19          |
| (1,1173) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB3  | 6        | 0.19          |
| (1,1173) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB3  | 6        | 0.19          |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 8        | 0.19          |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 8        | 0.19          |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 8        | 0.19          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 1        | 0.19          |
| (1,1143) | 1:157:A:LEU:HA   | 1:157:A:LEU:HB2  | 8        | 0.19          |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 1        | 0.19          |
| (1,1104) | 1:155:A:SER:HA   | 1:156:A:SER:HB3  | 3        | 0.19          |
| (1,1097) | 1:154:A:SER:HB3  | 1:155:A:SER:HA   | 8        | 0.19          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 6        | 0.19          |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG11 | 5        | 0.19          |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG12 | 5        | 0.19          |
| (1,987)  | 1:148:A:VAL:HA   | 1:153:A:VAL:HG13 | 5        | 0.19          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 10       | 0.19          |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 1        | 0.19          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 9        | 0.19          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 9        | 0.19          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 9        | 0.19          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 9        | 0.19          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 9        | 0.19          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 9        | 0.19          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG11 | 4        | 0.19          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG12 | 4        | 0.19          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG13 | 4        | 0.19          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG11 | 4        | 0.19          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG12 | 4        | 0.19          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG13 | 4        | 0.19          |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 7        | 0.19          |
| (1,782)  | 1:131:A:HIS:HB2  | 1:132:A:GLY:HA2  | 4        | 0.19          |
| (1,766)  | 1:129:A:ASP:HA   | 1:130:A:GLU:HB3  | 6        | 0.19          |
| (1,751)  | 1:128:A:GLN:HA   | 1:134:A:ILE:HD11 | 3        | 0.19          |
| (1,751)  | 1:128:A:GLN:HA   | 1:134:A:ILE:HD12 | 3        | 0.19          |
| (1,751)  | 1:128:A:GLN:HA   | 1:134:A:ILE:HD13 | 3        | 0.19          |
| (1,680)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 2        | 0.19          |
| (1,618)  | 1:119:A:GLU:HG2  | 1:141:A:LYS:HG3  | 6        | 0.19          |
| (1,610)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HD3  | 10       | 0.19          |
| (1,562)  | 1:117:A:VAL:HG11 | 1:142:A:TYR:HB3  | 1        | 0.19          |
| (1,562)  | 1:117:A:VAL:HG12 | 1:142:A:TYR:HB3  | 1        | 0.19          |
| (1,562)  | 1:117:A:VAL:HG13 | 1:142:A:TYR:HB3  | 1        | 0.19          |
| (1,521)  | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 8        | 0.19          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,521) | 1:116:A:GLY:HA2 | 1:118:A:VAL:HG22 | 8        | 0.19          |
| (1,521) | 1:116:A:GLY:HA2 | 1:118:A:VAL:HG23 | 8        | 0.19          |
| (1,419) | 1:111:A:VAL:HA  | 1:120:A:ILE:HG13 | 4        | 0.19          |
| (1,419) | 1:111:A:VAL:HA  | 1:120:A:ILE:HG13 | 9        | 0.19          |
| (1,349) | 1:109:A:LEU:HA  | 1:109:A:LEU:HB2  | 8        | 0.19          |
| (1,348) | 1:108:A:GLU:HG3 | 1:123:A:LYS:HE3  | 2        | 0.19          |
| (1,337) | 1:108:A:GLU:HA  | 1:108:A:GLU:HG3  | 5        | 0.19          |
| (1,306) | 1:106:A:PRO:HA  | 1:106:A:PRO:HB3  | 7        | 0.19          |
| (1,306) | 1:106:A:PRO:HA  | 1:106:A:PRO:HB3  | 8        | 0.19          |
| (1,280) | 1:102:A:ASN:HB3 | 1:161:A:GLY:HA3  | 7        | 0.19          |
| (1,279) | 1:102:A:ASN:HB3 | 1:161:A:GLY:HA2  | 4        | 0.19          |
| (1,269) | 1:101:A:VAL:HB  | 1:157:A:LEU:HD11 | 10       | 0.19          |
| (1,269) | 1:101:A:VAL:HB  | 1:157:A:LEU:HD12 | 10       | 0.19          |
| (1,269) | 1:101:A:VAL:HB  | 1:157:A:LEU:HD13 | 10       | 0.19          |
| (1,256) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HB   | 8        | 0.19          |
| (1,256) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HB   | 8        | 0.19          |
| (1,256) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HB   | 8        | 0.19          |
| (1,240) | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG11 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG12 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG13 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG11 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG12 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG13 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG11 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG12 | 1        | 0.19          |
| (1,240) | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG13 | 1        | 0.19          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG11 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG12 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG13 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG11 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG12 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG13 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG11 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG12 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG13 | 7        | 0.19          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG11 | 10       | 0.19          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG12 | 10       | 0.19          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG13 | 10       | 0.19          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG11 | 10       | 0.19          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG12 | 10       | 0.19          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG13 | 10       | 0.19          |
| (1,229) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG11 | 10       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG12 | 10       | 0.19          |
| (1,229)  | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG13 | 10       | 0.19          |
| (1,112)  | 1:96:A:ARG:HD3   | 1:164:A:THR:HA   | 2        | 0.19          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG21 | 6        | 0.19          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG22 | 6        | 0.19          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG23 | 6        | 0.19          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG21 | 7        | 0.19          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG22 | 7        | 0.19          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG23 | 7        | 0.19          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG21 | 2        | 0.19          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG22 | 2        | 0.19          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG23 | 2        | 0.19          |
| (1,48)   | 1:94:A:ARG:HD2   | 1:168:A:PRO:HA   | 7        | 0.19          |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 9        | 0.19          |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 10       | 0.19          |
| (1,17)   | 1:93:A:ASP:HA    | 1:169:A:MET:HG2  | 4        | 0.19          |
| (1,9)    | 1:90:A:HIS:HB3   | 1:91:A:THR:HA    | 9        | 0.19          |
| (1,4286) | 1:171:B:LYS:H    | 1:170:B:PRO:HB2  | 4        | 0.18          |
| (1,4267) | 1:167:B:ALA:H    | 1:169:B:MET:H    | 5        | 0.18          |
| (1,4196) | 1:162:B:THR:H    | 1:102:B:ASN:HB2  | 4        | 0.18          |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG21 | 9        | 0.18          |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG22 | 9        | 0.18          |
| (1,4195) | 1:161:B:GLY:H    | 1:162:B:THR:HG23 | 9        | 0.18          |
| (1,4194) | 1:161:B:GLY:H    | 1:162:B:THR:HB   | 9        | 0.18          |
| (1,4149) | 1:157:B:LEU:H    | 1:155:B:SER:HB2  | 10       | 0.18          |
| (1,4125) | 1:154:B:SER:H    | 1:168:B:PRO:HD2  | 7        | 0.18          |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB1  | 10       | 0.18          |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB2  | 10       | 0.18          |
| (1,4124) | 1:154:B:SER:H    | 1:167:B:ALA:HB3  | 10       | 0.18          |
| (1,4086) | 1:152:B:GLN:HE21 | 1:170:B:PRO:HD3  | 10       | 0.18          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 8        | 0.18          |
| (1,4076) | 1:152:B:GLN:H    | 1:170:B:PRO:HD3  | 7        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 4        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 4        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 4        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 5        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 5        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 5        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 6        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 6        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 6        | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 10       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 10       | 0.18          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 10       | 0.18          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD21  | 2        | 0.18          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD22  | 2        | 0.18          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD23  | 2        | 0.18          |
| (1,3952) | 1:136:B:ARG:H    | 1:135:B:SER:HB3  | 4        | 0.18          |
| (1,3936) | 1:134:B:ILE:H    | 1:127:B:ARG:HG2  | 9        | 0.18          |
| (1,3903) | 1:129:B:ASP:H    | 1:129:B:ASP:HB3  | 10       | 0.18          |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 5        | 0.18          |
| (1,3887) | 1:128:B:GLN:H    | 1:133:B:TYR:HD1  | 7        | 0.18          |
| (1,3887) | 1:128:B:GLN:H    | 1:133:B:TYR:HD2  | 7        | 0.18          |
| (1,3868) | 1:126:B:GLU:H    | 1:125:B:GLU:HG2  | 9        | 0.18          |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD21 | 4        | 0.18          |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD22 | 4        | 0.18          |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD23 | 4        | 0.18          |
| (1,3849) | 1:123:B:LYS:H    | 1:109:B:LEU:HD11 | 6        | 0.18          |
| (1,3849) | 1:123:B:LYS:H    | 1:109:B:LEU:HD12 | 6        | 0.18          |
| (1,3849) | 1:123:B:LYS:H    | 1:109:B:LEU:HD13 | 6        | 0.18          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD11 | 7        | 0.18          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD12 | 7        | 0.18          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD13 | 7        | 0.18          |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 3        | 0.18          |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 7        | 0.18          |
| (1,3748) | 1:113:B:THR:H    | 1:112:B:LYS:HB2  | 6        | 0.18          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 1        | 0.18          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 1        | 0.18          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 1        | 0.18          |
| (1,3681) | 1:107:B:ASP:H    | 1:106:B:PRO:HB3  | 4        | 0.18          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD11 | 1        | 0.18          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD12 | 1        | 0.18          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD13 | 1        | 0.18          |
| (1,3663) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA2  | 4        | 0.18          |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD11 | 8        | 0.18          |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD12 | 8        | 0.18          |
| (1,3652) | 1:102:B:ASN:HD21 | 1:157:B:LEU:HD13 | 8        | 0.18          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG21 | 9        | 0.18          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG22 | 9        | 0.18          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG23 | 9        | 0.18          |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 3        | 0.18          |
| (1,3491) | 1:160:B:GLU:HB2  | 1:162:B:THR:HB   | 3        | 0.18          |
| (1,3309) | 1:149:B:ASP:HA   | 1:150:B:PRO:HD3  | 3        | 0.18          |
| (1,3304) | 1:149:B:ASP:HA   | 1:149:B:ASP:HB3  | 3        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 8        | 0.18          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 8        | 0.18          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 8        | 0.18          |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 3        | 0.18          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG11 | 4        | 0.18          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG12 | 4        | 0.18          |
| (1,3234) | 1:145:B:PRO:HB3  | 1:148:B:VAL:HG13 | 4        | 0.18          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 10       | 0.18          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 10       | 0.18          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 8        | 0.18          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 8        | 0.18          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 8        | 0.18          |
| (1,3112) | 1:139:B:THR:HB   | 1:141:B:LYS:HE2  | 9        | 0.18          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD1  | 4        | 0.18          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD2  | 4        | 0.18          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD1  | 4        | 0.18          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD2  | 4        | 0.18          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD1  | 4        | 0.18          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD2  | 4        | 0.18          |
| (1,3060) | 1:131:B:HIS:HA   | 1:131:B:HIS:HE1  | 4        | 0.18          |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD1  | 7        | 0.18          |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD2  | 7        | 0.18          |
| (1,3003) | 1:126:B:GLU:HG2  | 1:135:B:SER:HA   | 7        | 0.18          |
| (1,3000) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HD1  | 2        | 0.18          |
| (1,3000) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HD2  | 2        | 0.18          |
| (1,2996) | 1:126:B:GLU:HB2  | 1:135:B:SER:HB3  | 10       | 0.18          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 1        | 0.18          |
| (1,2957) | 1:122:B:GLY:HA3  | 1:137:B:CYS:HA   | 6        | 0.18          |
| (1,2892) | 1:119:B:GLU:HA   | 1:141:B:LYS:HE2  | 1        | 0.18          |
| (1,2891) | 1:119:B:GLU:HA   | 1:141:B:LYS:HD3  | 7        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 1        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 1        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 1        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 1        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 1        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 1        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 1        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 1        | 0.18          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 1        | 0.18          |
| (1,2852) | 1:118:B:VAL:HB   | 1:142:B:TYR:HD1  | 2        | 0.18          |
| (1,2852) | 1:118:B:VAL:HB   | 1:142:B:TYR:HD2  | 2        | 0.18          |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 9        | 0.18          |
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 9        | 0.18          |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 9        | 0.18          |
| (1,2734) | 1:112:B:LYS:HA   | 1:114:B:LYS:HB3  | 3        | 0.18          |
| (1,2687) | 1:110:B:THR:HG21 | 1:112:B:LYS:HE3  | 4        | 0.18          |
| (1,2687) | 1:110:B:THR:HG22 | 1:112:B:LYS:HE3  | 4        | 0.18          |
| (1,2687) | 1:110:B:THR:HG23 | 1:112:B:LYS:HE3  | 4        | 0.18          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 3        | 0.18          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 3        | 0.18          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 3        | 0.18          |
| (1,2618) | 1:108:B:GLU:HA   | 1:108:B:GLU:HG3  | 2        | 0.18          |
| (1,2596) | 1:106:B:PRO:HA   | 1:157:B:LEU:HB2  | 2        | 0.18          |
| (1,2587) | 1:106:B:PRO:HA   | 1:106:B:PRO:HB3  | 4        | 0.18          |
| (1,2578) | 1:105:B:ALA:HB1  | 1:107:B:ASP:HB3  | 4        | 0.18          |
| (1,2578) | 1:105:B:ALA:HB2  | 1:107:B:ASP:HB3  | 4        | 0.18          |
| (1,2578) | 1:105:B:ALA:HB3  | 1:107:B:ASP:HB3  | 4        | 0.18          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 3        | 0.18          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 3        | 0.18          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 3        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD11 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD12 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD13 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD11 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD12 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD13 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD11 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD12 | 2        | 0.18          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD13 | 2        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 3        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 3        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 3        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 3        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 3        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 3        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 3        | 0.18          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 3        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 3        | 0.18          |
| (1,2467) | 1:98:B:SER:HB2   | 1:164:B:THR:HA   | 7        | 0.18          |
| (1,2442) | 1:97:B:VAL:HG21  | 1:166:B:GLU:HA   | 1        | 0.18          |
| (1,2442) | 1:97:B:VAL:HG22  | 1:166:B:GLU:HA   | 1        | 0.18          |
| (1,2442) | 1:97:B:VAL:HG23  | 1:166:B:GLU:HA   | 1        | 0.18          |
| (1,2442) | 1:97:B:VAL:HG21  | 1:166:B:GLU:HA   | 2        | 0.18          |
| (1,2442) | 1:97:B:VAL:HG22  | 1:166:B:GLU:HA   | 2        | 0.18          |
| (1,2442) | 1:97:B:VAL:HG23  | 1:166:B:GLU:HA   | 2        | 0.18          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG21 | 1        | 0.18          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG22 | 1        | 0.18          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG23 | 1        | 0.18          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 9        | 0.18          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 9        | 0.18          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 9        | 0.18          |
| (1,2361) | 1:96:B:ARG:HA    | 1:96:B:ARG:HD3   | 8        | 0.18          |
| (1,2332) | 1:95:B:TRP:HA    | 1:95:B:TRP:HB2   | 7        | 0.18          |
| (1,2326) | 1:94:B:ARG:HG2   | 1:168:B:PRO:HB2  | 5        | 0.18          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 6        | 0.18          |
| (1,2310) | 1:94:B:ARG:HA    | 1:168:B:PRO:HA   | 5        | 0.18          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 9        | 0.18          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 9        | 0.18          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 9        | 0.18          |
| (1,2152) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 7        | 0.18          |
| (1,2152) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 7        | 0.18          |
| (1,2152) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 7        | 0.18          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 9        | 0.18          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 9        | 0.18          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 9        | 0.18          |
| (1,2020) | 1:97:A:VAL:HG11  | 1:131:B:HIS:HB3  | 7        | 0.18          |
| (1,2020) | 1:97:A:VAL:HG12  | 1:131:B:HIS:HB3  | 7        | 0.18          |
| (1,2020) | 1:97:A:VAL:HG13  | 1:131:B:HIS:HB3  | 7        | 0.18          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 8        | 0.18          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 9        | 0.18          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 5        | 0.18          |
| (1,1920) | 1:162:A:THR:H    | 1:158:A:SER:HB2  | 2        | 0.18          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 4        | 0.18          |
| (1,1910) | 1:161:A:GLY:H    | 1:160:A:GLU:HG3  | 8        | 0.18          |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB1  | 3        | 0.18          |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB2  | 3        | 0.18          |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB3  | 3        | 0.18          |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 5        | 0.18          |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 7        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1655) | 1:134:A:ILE:H    | 1:127:A:ARG:HG2  | 6        | 0.18          |
| (1,1655) | 1:134:A:ILE:H    | 1:127:A:ARG:HG2  | 10       | 0.18          |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 5        | 0.18          |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 10       | 0.18          |
| (1,1597) | 1:128:A:GLN:H    | 1:127:A:ARG:HB3  | 7        | 0.18          |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 1        | 0.18          |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 6        | 0.18          |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 8        | 0.18          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 6        | 0.18          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 10       | 0.18          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 10       | 0.18          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 10       | 0.18          |
| (1,1391) | 1:105:A:ALA:H    | 1:108:A:GLU:HB3  | 1        | 0.18          |
| (1,1391) | 1:105:A:ALA:H    | 1:108:A:GLU:HB3  | 7        | 0.18          |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD11 | 1        | 0.18          |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD12 | 1        | 0.18          |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD13 | 1        | 0.18          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD11 | 5        | 0.18          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD12 | 5        | 0.18          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD13 | 5        | 0.18          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG21 | 9        | 0.18          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG22 | 9        | 0.18          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG23 | 9        | 0.18          |
| (1,1304) | 1:169:A:MET:HG3  | 1:170:A:PRO:HD2  | 10       | 0.18          |
| (1,1276) | 1:168:A:PRO:HA   | 1:169:A:MET:HG2  | 6        | 0.18          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD21 | 6        | 0.18          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD22 | 6        | 0.18          |
| (1,1218) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HD23 | 6        | 0.18          |
| (1,1206) | 1:159:A:PRO:HD2  | 1:160:A:GLU:HB3  | 7        | 0.18          |
| (1,1197) | 1:158:A:SER:HB3  | 1:159:A:PRO:HD3  | 7        | 0.18          |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 5        | 0.18          |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 5        | 0.18          |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 5        | 0.18          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG21 | 4        | 0.18          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG22 | 4        | 0.18          |
| (1,1100) | 1:154:A:SER:HB2  | 1:165:A:VAL:HG23 | 4        | 0.18          |
| (1,1065) | 1:152:A:GLN:HB2  | 1:169:A:MET:HA   | 6        | 0.18          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 2        | 0.18          |
| (1,1014) | 1:148:A:VAL:HG11 | 1:170:A:PRO:HG3  | 6        | 0.18          |
| (1,1014) | 1:148:A:VAL:HG12 | 1:170:A:PRO:HG3  | 6        | 0.18          |
| (1,1014) | 1:148:A:VAL:HG13 | 1:170:A:PRO:HG3  | 6        | 0.18          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 2        | 0.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,962) | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 4        | 0.18          |
| (1,962) | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 7        | 0.18          |
| (1,938) | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG21 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG22 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG23 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG21 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG22 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG23 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG21 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG22 | 6        | 0.18          |
| (1,938) | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG23 | 6        | 0.18          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 4        | 0.18          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 4        | 0.18          |
| (1,896) | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 4        | 0.18          |
| (1,856) | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 8        | 0.18          |
| (1,849) | 1:141:A:LYS:HB2  | 1:141:A:LYS:HE2  | 6        | 0.18          |
| (1,842) | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 2        | 0.18          |
| (1,749) | 1:128:A:GLN:HA   | 1:133:A:TYR:HE1  | 1        | 0.18          |
| (1,749) | 1:128:A:GLN:HA   | 1:133:A:TYR:HE2  | 1        | 0.18          |
| (1,664) | 1:121:A:THR:HA   | 1:139:A:THR:HA   | 2        | 0.18          |
| (1,664) | 1:121:A:THR:HA   | 1:139:A:THR:HA   | 9        | 0.18          |
| (1,614) | 1:119:A:GLU:HB3  | 1:139:A:THR:HA   | 1        | 0.18          |
| (1,562) | 1:117:A:VAL:HG11 | 1:142:A:TYR:HB3  | 8        | 0.18          |
| (1,562) | 1:117:A:VAL:HG12 | 1:142:A:TYR:HB3  | 8        | 0.18          |
| (1,562) | 1:117:A:VAL:HG13 | 1:142:A:TYR:HB3  | 8        | 0.18          |
| (1,558) | 1:117:A:VAL:HG11 | 1:141:A:LYS:HE2  | 1        | 0.18          |
| (1,558) | 1:117:A:VAL:HG12 | 1:141:A:LYS:HE2  | 1        | 0.18          |
| (1,558) | 1:117:A:VAL:HG13 | 1:141:A:LYS:HE2  | 1        | 0.18          |
| (1,509) | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 9        | 0.18          |
| (1,457) | 1:112:A:LYS:HB2  | 1:120:A:ILE:HA   | 7        | 0.18          |
| (1,418) | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 3        | 0.18          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD11 | 10       | 0.18          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD12 | 10       | 0.18          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD13 | 10       | 0.18          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD11 | 10       | 0.18          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD12 | 10       | 0.18          |
| (1,358) | 1:109:A:LEU:HB2  | 1:109:A:LEU:HD13 | 10       | 0.18          |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 1        | 0.18          |
| (1,349) | 1:109:A:LEU:HA   | 1:109:A:LEU:HB2  | 10       | 0.18          |
| (1,337) | 1:108:A:GLU:HA   | 1:108:A:GLU:HG3  | 7        | 0.18          |
| (1,315) | 1:106:A:PRO:HA   | 1:157:A:LEU:HB2  | 4        | 0.18          |
| (1,296) | 1:105:A:ALA:HB1  | 1:107:A:ASP:HB2  | 7        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,296)  | 1:105:A:ALA:HB2 | 1:107:A:ASP:HB2  | 7        | 0.18          |
| (1,296)  | 1:105:A:ALA:HB3 | 1:107:A:ASP:HB2  | 7        | 0.18          |
| (1,296)  | 1:105:A:ALA:HB1 | 1:107:A:ASP:HB2  | 9        | 0.18          |
| (1,296)  | 1:105:A:ALA:HB2 | 1:107:A:ASP:HB2  | 9        | 0.18          |
| (1,296)  | 1:105:A:ALA:HB3 | 1:107:A:ASP:HB2  | 9        | 0.18          |
| (1,283)  | 1:105:A:ALA:HA  | 1:106:A:PRO:HB3  | 5        | 0.18          |
| (1,283)  | 1:105:A:ALA:HA  | 1:106:A:PRO:HB3  | 9        | 0.18          |
| (1,280)  | 1:102:A:ASN:HB3 | 1:161:A:GLY:HA3  | 9        | 0.18          |
| (1,279)  | 1:102:A:ASN:HB3 | 1:161:A:GLY:HA2  | 2        | 0.18          |
| (1,276)  | 1:102:A:ASN:HB2 | 1:157:A:LEU:HD11 | 2        | 0.18          |
| (1,276)  | 1:102:A:ASN:HB2 | 1:157:A:LEU:HD12 | 2        | 0.18          |
| (1,276)  | 1:102:A:ASN:HB2 | 1:157:A:LEU:HD13 | 2        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG11 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG12 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG13 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG11 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG12 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG13 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG11 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG12 | 3        | 0.18          |
| (1,240)  | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG13 | 3        | 0.18          |
| (1,237)  | 1:99:A:LEU:HD21 | 1:101:A:VAL:HB   | 8        | 0.18          |
| (1,237)  | 1:99:A:LEU:HD22 | 1:101:A:VAL:HB   | 8        | 0.18          |
| (1,237)  | 1:99:A:LEU:HD23 | 1:101:A:VAL:HB   | 8        | 0.18          |
| (1,166)  | 1:97:A:VAL:HG11 | 1:118:A:VAL:HB   | 6        | 0.18          |
| (1,166)  | 1:97:A:VAL:HG12 | 1:118:A:VAL:HB   | 6        | 0.18          |
| (1,166)  | 1:97:A:VAL:HG13 | 1:118:A:VAL:HB   | 6        | 0.18          |
| (1,129)  | 1:97:A:VAL:HB   | 1:148:A:VAL:HG11 | 8        | 0.18          |
| (1,129)  | 1:97:A:VAL:HB   | 1:148:A:VAL:HG12 | 8        | 0.18          |
| (1,129)  | 1:97:A:VAL:HB   | 1:148:A:VAL:HG13 | 8        | 0.18          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG21 | 10       | 0.18          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG22 | 10       | 0.18          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG23 | 10       | 0.18          |
| (1,45)   | 1:94:A:ARG:HG2  | 1:168:A:PRO:HB2  | 7        | 0.18          |
| (1,9)    | 1:90:A:HIS:HB3  | 1:91:A:THR:HA    | 8        | 0.18          |
| (1,6)    | 1:90:A:HIS:HA   | 1:91:A:THR:HG21  | 7        | 0.18          |
| (1,6)    | 1:90:A:HIS:HA   | 1:91:A:THR:HG22  | 7        | 0.18          |
| (1,6)    | 1:90:A:HIS:HA   | 1:91:A:THR:HG23  | 7        | 0.18          |
| (1,4197) | 1:162:B:THR:H   | 1:102:B:ASN:HB3  | 3        | 0.17          |
| (1,4194) | 1:161:B:GLY:H   | 1:162:B:THR:HB   | 1        | 0.17          |
| (1,4192) | 1:161:B:GLY:H   | 1:161:B:GLY:HA2  | 4        | 0.17          |
| (1,4192) | 1:161:B:GLY:H   | 1:161:B:GLY:HA2  | 10       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 3        | 0.17          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 3        | 0.17          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 3        | 0.17          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD11  | 4        | 0.17          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD12  | 4        | 0.17          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD13  | 4        | 0.17          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD21  | 8        | 0.17          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD22  | 8        | 0.17          |
| (1,3971) | 1:140:B:ARG:H    | 1:99:B:LEU:HD23  | 8        | 0.17          |
| (1,3910) | 1:129:B:ASP:H    | 1:133:B:TYR:HB2  | 6        | 0.17          |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 2        | 0.17          |
| (1,3878) | 1:128:B:GLN:H    | 1:127:B:ARG:HB3  | 9        | 0.17          |
| (1,3869) | 1:126:B:GLU:H    | 1:125:B:GLU:HG3  | 7        | 0.17          |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB1  | 9        | 0.17          |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB2  | 9        | 0.17          |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB3  | 9        | 0.17          |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 6        | 0.17          |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 3        | 0.17          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 7        | 0.17          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 7        | 0.17          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 7        | 0.17          |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD12 | 4        | 0.17          |
| (1,3689) | 1:107:B:ASP:H    | 1:109:B:LEU:HD13 | 5        | 0.17          |
| (1,3663) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA2  | 7        | 0.17          |
| (1,3648) | 1:102:B:ASN:H    | 1:102:B:ASN:HD21 | 10       | 0.17          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG21 | 10       | 0.17          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG22 | 10       | 0.17          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG23 | 10       | 0.17          |
| (1,3569) | 1:169:B:MET:HA   | 1:169:B:MET:HG2  | 7        | 0.17          |
| (1,3460) | 1:157:B:LEU:HD21 | 1:163:B:LEU:HB3  | 10       | 0.17          |
| (1,3460) | 1:157:B:LEU:HD22 | 1:163:B:LEU:HB3  | 10       | 0.17          |
| (1,3460) | 1:157:B:LEU:HD23 | 1:163:B:LEU:HB3  | 10       | 0.17          |
| (1,3455) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HG   | 5        | 0.17          |
| (1,3455) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HG   | 5        | 0.17          |
| (1,3455) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HG   | 5        | 0.17          |
| (1,3454) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB3  | 2        | 0.17          |
| (1,3454) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB3  | 2        | 0.17          |
| (1,3454) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB3  | 2        | 0.17          |
| (1,3454) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB3  | 10       | 0.17          |
| (1,3454) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB3  | 10       | 0.17          |
| (1,3454) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB3  | 10       | 0.17          |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 6        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 6        | 0.17          |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 6        | 0.17          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD21 | 5        | 0.17          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD22 | 5        | 0.17          |
| (1,3422) | 1:156:B:SER:HB3  | 1:163:B:LEU:HD23 | 5        | 0.17          |
| (1,3391) | 1:155:B:SER:HA   | 1:165:B:VAL:HA   | 1        | 0.17          |
| (1,3358) | 1:153:B:VAL:HA   | 1:168:B:PRO:HD2  | 9        | 0.17          |
| (1,3336) | 1:151:B:THR:HB   | 1:153:B:VAL:HG21 | 5        | 0.17          |
| (1,3336) | 1:151:B:THR:HB   | 1:153:B:VAL:HG22 | 5        | 0.17          |
| (1,3336) | 1:151:B:THR:HB   | 1:153:B:VAL:HG23 | 5        | 0.17          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 4        | 0.17          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 8        | 0.17          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 10       | 0.17          |
| (1,3302) | 1:148:B:VAL:HG21 | 1:169:B:MET:HB3  | 2        | 0.17          |
| (1,3302) | 1:148:B:VAL:HG22 | 1:169:B:MET:HB3  | 2        | 0.17          |
| (1,3302) | 1:148:B:VAL:HG23 | 1:169:B:MET:HB3  | 2        | 0.17          |
| (1,3295) | 1:148:B:VAL:HG11 | 1:170:B:PRO:HG3  | 6        | 0.17          |
| (1,3295) | 1:148:B:VAL:HG12 | 1:170:B:PRO:HG3  | 6        | 0.17          |
| (1,3295) | 1:148:B:VAL:HG13 | 1:170:B:PRO:HG3  | 6        | 0.17          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 2        | 0.17          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 2        | 0.17          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 2        | 0.17          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG11 | 4        | 0.17          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG12 | 4        | 0.17          |
| (1,3268) | 1:148:B:VAL:HA   | 1:153:B:VAL:HG13 | 4        | 0.17          |
| (1,3252) | 1:146:B:PRO:HG2  | 1:147:B:GLY:HA2  | 10       | 0.17          |
| (1,3249) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA3  | 3        | 0.17          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 6        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 7        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG21 | 8        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG22 | 8        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD21 | 1:148:B:VAL:HG23 | 8        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG21 | 8        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG22 | 8        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3219) | 1:144:B:LEU:HD22 | 1:148:B:VAL:HG23 | 8        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG21 | 8        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG22 | 8        | 0.17          |
| (1,3219) | 1:144:B:LEU:HD23 | 1:148:B:VAL:HG23 | 8        | 0.17          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 1        | 0.17          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 1        | 0.17          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 1        | 0.17          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 2        | 0.17          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 2        | 0.17          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 2        | 0.17          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 9        | 0.17          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 9        | 0.17          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 9        | 0.17          |
| (1,3138) | 1:141:B:LYS:HG2  | 1:143:B:THR:HA   | 8        | 0.17          |
| (1,3133) | 1:141:B:LYS:HG2  | 1:141:B:LYS:HE2  | 7        | 0.17          |
| (1,3130) | 1:141:B:LYS:HB2  | 1:141:B:LYS:HE2  | 9        | 0.17          |
| (1,3027) | 1:128:B:GLN:HA   | 1:128:B:GLN:HG3  | 8        | 0.17          |
| (1,3014) | 1:126:B:GLU:HG3  | 1:135:B:SER:HB3  | 2        | 0.17          |
| (1,3000) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HD1  | 3        | 0.17          |
| (1,3000) | 1:126:B:GLU:HG2  | 1:133:B:TYR:HD2  | 3        | 0.17          |
| (1,2945) | 1:121:B:THR:HA   | 1:139:B:THR:HA   | 8        | 0.17          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 6        | 0.17          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 6        | 0.17          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 6        | 0.17          |
| (1,2831) | 1:117:B:VAL:HA   | 1:148:B:VAL:HB   | 8        | 0.17          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG21 | 4        | 0.17          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG22 | 4        | 0.17          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG23 | 4        | 0.17          |
| (1,2790) | 1:114:B:LYS:HA   | 1:114:B:LYS:HB2  | 1        | 0.17          |
| (1,2716) | 1:111:B:VAL:HG21 | 1:120:B:ILE:HG13 | 1        | 0.17          |
| (1,2716) | 1:111:B:VAL:HG22 | 1:120:B:ILE:HG13 | 1        | 0.17          |
| (1,2716) | 1:111:B:VAL:HG23 | 1:120:B:ILE:HG13 | 1        | 0.17          |
| (1,2700) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG13 | 2        | 0.17          |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 7        | 0.17          |
| (1,2664) | 1:109:B:LEU:HD21 | 1:122:B:GLY:HA3  | 1        | 0.17          |
| (1,2664) | 1:109:B:LEU:HD22 | 1:122:B:GLY:HA3  | 1        | 0.17          |
| (1,2664) | 1:109:B:LEU:HD23 | 1:122:B:GLY:HA3  | 1        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 5        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 5        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 5        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 5        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 5        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 5        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 5        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 5        | 0.17          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 5        | 0.17          |
| (1,2619) | 1:108:B:GLU:HA   | 1:123:B:LYS:HD2  | 4        | 0.17          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 7        | 0.17          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 7        | 0.17          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 7        | 0.17          |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 6        | 0.17          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD11 | 7        | 0.17          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD12 | 7        | 0.17          |
| (1,2550) | 1:101:B:VAL:HB   | 1:157:B:LEU:HD13 | 7        | 0.17          |
| (1,2546) | 1:100:B:ASP:HB3  | 1:162:B:THR:HA   | 2        | 0.17          |
| (1,2518) | 1:99:B:LEU:HD21  | 1:101:B:VAL:HB   | 3        | 0.17          |
| (1,2518) | 1:99:B:LEU:HD22  | 1:101:B:VAL:HB   | 3        | 0.17          |
| (1,2518) | 1:99:B:LEU:HD23  | 1:101:B:VAL:HB   | 3        | 0.17          |
| (1,2518) | 1:99:B:LEU:HD21  | 1:101:B:VAL:HB   | 5        | 0.17          |
| (1,2518) | 1:99:B:LEU:HD22  | 1:101:B:VAL:HB   | 5        | 0.17          |
| (1,2518) | 1:99:B:LEU:HD23  | 1:101:B:VAL:HB   | 5        | 0.17          |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 3        | 0.17          |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 3        | 0.17          |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 3        | 0.17          |
| (1,2397) | 1:96:B:ARG:HD2   | 1:166:B:GLU:HB3  | 10       | 0.17          |
| (1,2394) | 1:96:B:ARG:HD2   | 1:164:B:THR:HB   | 1        | 0.17          |
| (1,2301) | 1:93:B:ASP:HB3   | 1:94:B:ARG:HA    | 4        | 0.17          |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG21  | 7        | 0.17          |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG22  | 7        | 0.17          |
| (1,2289) | 1:90:B:HIS:HB2   | 1:91:B:THR:HG23  | 7        | 0.17          |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 4        | 0.17          |
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 4        | 0.17          |
| (1,2013) | 1:172:A:LEU:H    | 1:172:A:LEU:HB2  | 3        | 0.17          |
| (1,1998) | 1:169:A:MET:H    | 1:169:A:MET:HB2  | 6        | 0.17          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 7        | 0.17          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG21 | 3        | 0.17          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG22 | 3        | 0.17          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG23 | 3        | 0.17          |
| (1,1901) | 1:161:A:GLY:H    | 1:102:A:ASN:HB2  | 9        | 0.17          |
| (1,1799) | 1:152:A:GLN:HE21 | 1:152:A:GLN:HB3  | 5        | 0.17          |
| (1,1756) | 1:148:A:VAL:H    | 1:170:A:PRO:HG3  | 6        | 0.17          |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 2        | 0.17          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 8        | 0.17          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 8        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 8        | 0.17          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 8        | 0.17          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 8        | 0.17          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 8        | 0.17          |
| (1,1634) | 1:131:A:HIS:H    | 1:129:A:ASP:HB3  | 5        | 0.17          |
| (1,1634) | 1:131:A:HIS:H    | 1:129:A:ASP:HB3  | 6        | 0.17          |
| (1,1588) | 1:126:A:GLU:H    | 1:125:A:GLU:HG3  | 6        | 0.17          |
| (1,1525) | 1:119:A:GLU:H    | 1:114:A:LYS:HB3  | 6        | 0.17          |
| (1,1525) | 1:119:A:GLU:H    | 1:114:A:LYS:HB3  | 9        | 0.17          |
| (1,1489) | 1:114:A:LYS:H    | 1:119:A:GLU:H    | 3        | 0.17          |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 5        | 0.17          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 2        | 0.17          |
| (1,1391) | 1:105:A:ALA:H    | 1:108:A:GLU:HB3  | 6        | 0.17          |
| (1,1389) | 1:105:A:ALA:H    | 1:106:A:PRO:HD3  | 3        | 0.17          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD21 | 10       | 0.17          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD22 | 10       | 0.17          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD23 | 10       | 0.17          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD11 | 1        | 0.17          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD12 | 1        | 0.17          |
| (1,1380) | 1:102:A:ASN:HD22 | 1:157:A:LEU:HD13 | 1        | 0.17          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 2        | 0.17          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 5        | 0.17          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 3        | 0.17          |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 9        | 0.17          |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 9        | 0.17          |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 9        | 0.17          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 6        | 0.17          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 1        | 0.17          |
| (1,1104) | 1:155:A:SER:HA   | 1:156:A:SER:HB3  | 6        | 0.17          |
| (1,1064) | 1:152:A:GLN:HB2  | 1:168:A:PRO:HD3  | 4        | 0.17          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG21 | 7        | 0.17          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG22 | 7        | 0.17          |
| (1,1046) | 1:150:A:PRO:HD2  | 1:151:A:THR:HG23 | 7        | 0.17          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 1        | 0.17          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 5        | 0.17          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 4        | 0.17          |
| (1,992)  | 1:148:A:VAL:HA   | 1:170:A:PRO:HB3  | 7        | 0.17          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 7        | 0.17          |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 8        | 0.17          |
| (1,858)  | 1:141:A:LYS:HG3  | 1:141:A:LYS:HE2  | 4        | 0.17          |
| (1,842)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 7        | 0.17          |
| (1,747)  | 1:128:A:GLN:HA   | 1:133:A:TYR:HB2  | 10       | 0.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,726) | 1:126:A:GLU:HG3  | 1:127:A:ARG:HG2  | 7        | 0.17          |
| (1,680) | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 4        | 0.17          |
| (1,640) | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD11 | 9        | 0.17          |
| (1,640) | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD12 | 9        | 0.17          |
| (1,640) | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD13 | 9        | 0.17          |
| (1,611) | 1:119:A:GLU:HA   | 1:141:A:LYS:HE2  | 5        | 0.17          |
| (1,605) | 1:119:A:GLU:HA   | 1:120:A:ILE:HG13 | 8        | 0.17          |
| (1,602) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG3  | 5        | 0.17          |
| (1,602) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG3  | 6        | 0.17          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 3        | 0.17          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 3        | 0.17          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 3        | 0.17          |
| (1,478) | 1:112:A:LYS:HE2  | 1:121:A:THR:HB   | 1        | 0.17          |
| (1,436) | 1:111:A:VAL:HG21 | 1:120:A:ILE:HD11 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG21 | 1:120:A:ILE:HD12 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG21 | 1:120:A:ILE:HD13 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG22 | 1:120:A:ILE:HD11 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG22 | 1:120:A:ILE:HD12 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG22 | 1:120:A:ILE:HD13 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG23 | 1:120:A:ILE:HD11 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG23 | 1:120:A:ILE:HD12 | 4        | 0.17          |
| (1,436) | 1:111:A:VAL:HG23 | 1:120:A:ILE:HD13 | 4        | 0.17          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG21 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG22 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG23 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG21 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG22 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG23 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG21 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG22 | 6        | 0.17          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG23 | 6        | 0.17          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 10       | 0.17          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 10       | 0.17          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD21 | 2        | 0.17          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD22 | 2        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,361)  | 1:109:A:LEU:HB3 | 1:109:A:LEU:HD23 | 2        | 0.17          |
| (1,359)  | 1:109:A:LEU:HB2 | 1:122:A:GLY:HA2  | 7        | 0.17          |
| (1,335)  | 1:107:A:ASP:HA  | 1:157:A:LEU:HD21 | 4        | 0.17          |
| (1,335)  | 1:107:A:ASP:HA  | 1:157:A:LEU:HD22 | 4        | 0.17          |
| (1,335)  | 1:107:A:ASP:HA  | 1:157:A:LEU:HD23 | 4        | 0.17          |
| (1,331)  | 1:107:A:ASP:HA  | 1:108:A:GLU:HG2  | 6        | 0.17          |
| (1,289)  | 1:105:A:ALA:HA  | 1:157:A:LEU:HD11 | 4        | 0.17          |
| (1,289)  | 1:105:A:ALA:HA  | 1:157:A:LEU:HD12 | 4        | 0.17          |
| (1,289)  | 1:105:A:ALA:HA  | 1:157:A:LEU:HD13 | 4        | 0.17          |
| (1,279)  | 1:102:A:ASN:HB3 | 1:161:A:GLY:HA2  | 6        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG11 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG12 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD21 | 1:111:A:VAL:HG13 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG11 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG12 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD22 | 1:111:A:VAL:HG13 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG11 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG12 | 2        | 0.17          |
| (1,240)  | 1:99:A:LEU:HD23 | 1:111:A:VAL:HG13 | 2        | 0.17          |
| (1,216)  | 1:99:A:LEU:HB3  | 1:109:A:LEU:HD11 | 10       | 0.17          |
| (1,216)  | 1:99:A:LEU:HB3  | 1:109:A:LEU:HD12 | 10       | 0.17          |
| (1,216)  | 1:99:A:LEU:HB3  | 1:109:A:LEU:HD13 | 10       | 0.17          |
| (1,101)  | 1:96:A:ARG:HB3  | 1:166:A:GLU:HA   | 8        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG21 | 1        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG22 | 1        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG23 | 1        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG21 | 3        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG22 | 3        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG23 | 3        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG21 | 6        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG22 | 6        | 0.17          |
| (1,88)   | 1:96:A:ARG:HA   | 1:165:A:VAL:HG23 | 6        | 0.17          |
| (1,37)   | 1:94:A:ARG:HB2  | 1:96:A:ARG:HA    | 5        | 0.17          |
| (1,29)   | 1:94:A:ARG:HA   | 1:168:A:PRO:HA   | 6        | 0.17          |
| (1,23)   | 1:94:A:ARG:HA   | 1:94:A:ARG:HB3   | 8        | 0.17          |
| (1,4278) | 1:169:B:MET:H   | 1:169:B:MET:HA   | 5        | 0.16          |
| (1,4195) | 1:161:B:GLY:H   | 1:162:B:THR:HG21 | 5        | 0.16          |
| (1,4195) | 1:161:B:GLY:H   | 1:162:B:THR:HG22 | 5        | 0.16          |
| (1,4195) | 1:161:B:GLY:H   | 1:162:B:THR:HG23 | 5        | 0.16          |
| (1,4195) | 1:161:B:GLY:H   | 1:162:B:THR:HG21 | 10       | 0.16          |
| (1,4195) | 1:161:B:GLY:H   | 1:162:B:THR:HG22 | 10       | 0.16          |
| (1,4195) | 1:161:B:GLY:H   | 1:162:B:THR:HG23 | 10       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4192) | 1:161:B:GLY:H    | 1:161:B:GLY:HA2  | 8        | 0.16          |
| (1,4191) | 1:161:B:GLY:H    | 1:160:B:GLU:HG2  | 3        | 0.16          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 9        | 0.16          |
| (1,4182) | 1:161:B:GLY:H    | 1:102:B:ASN:HB2  | 1        | 0.16          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG21 | 9        | 0.16          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG22 | 9        | 0.16          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG23 | 9        | 0.16          |
| (1,4125) | 1:154:B:SER:H    | 1:168:B:PRO:HD2  | 3        | 0.16          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 10       | 0.16          |
| (1,4036) | 1:148:B:VAL:H    | 1:170:B:PRO:HB2  | 3        | 0.16          |
| (1,3984) | 1:142:B:TYR:H    | 1:141:B:LYS:HG2  | 6        | 0.16          |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG3  | 9        | 0.16          |
| (1,3907) | 1:129:B:ASP:H    | 1:132:B:GLY:HA3  | 2        | 0.16          |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD21 | 10       | 0.16          |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD22 | 10       | 0.16          |
| (1,3850) | 1:123:B:LYS:H    | 1:109:B:LEU:HD23 | 10       | 0.16          |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB1  | 5        | 0.16          |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB2  | 5        | 0.16          |
| (1,3844) | 1:123:B:LYS:H    | 1:105:B:ALA:HB3  | 5        | 0.16          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD11 | 2        | 0.16          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD12 | 2        | 0.16          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD13 | 2        | 0.16          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD11 | 9        | 0.16          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD12 | 9        | 0.16          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD13 | 9        | 0.16          |
| (1,3770) | 1:114:B:LYS:H    | 1:119:B:GLU:H    | 3        | 0.16          |
| (1,3770) | 1:114:B:LYS:H    | 1:119:B:GLU:H    | 10       | 0.16          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 4        | 0.16          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 4        | 0.16          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 4        | 0.16          |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD21 | 6        | 0.16          |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD22 | 6        | 0.16          |
| (1,3662) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD23 | 6        | 0.16          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG21 | 8        | 0.16          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG22 | 8        | 0.16          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG23 | 8        | 0.16          |
| (1,3569) | 1:169:B:MET:HA   | 1:169:B:MET:HG2  | 2        | 0.16          |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 4        | 0.16          |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 2        | 0.16          |
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 2        | 0.16          |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 2        | 0.16          |
| (1,3430) | 1:157:B:LEU:HA   | 1:163:B:LEU:HB3  | 5        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3360) | 1:153:B:VAL:HB   | 1:154:B:SER:HA   | 9        | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG21 | 7        | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG22 | 7        | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG23 | 7        | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG21 | 8        | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG22 | 8        | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG23 | 8        | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG21 | 10       | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG22 | 10       | 0.16          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG23 | 10       | 0.16          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 2        | 0.16          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 6        | 0.16          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 9        | 0.16          |
| (1,3292) | 1:148:B:VAL:HG11 | 1:169:B:MET:HA   | 1        | 0.16          |
| (1,3292) | 1:148:B:VAL:HG12 | 1:169:B:MET:HA   | 1        | 0.16          |
| (1,3292) | 1:148:B:VAL:HG13 | 1:169:B:MET:HA   | 1        | 0.16          |
| (1,3292) | 1:148:B:VAL:HG11 | 1:169:B:MET:HA   | 2        | 0.16          |
| (1,3292) | 1:148:B:VAL:HG12 | 1:169:B:MET:HA   | 2        | 0.16          |
| (1,3292) | 1:148:B:VAL:HG13 | 1:169:B:MET:HA   | 2        | 0.16          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 3        | 0.16          |
| (1,3243) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HG3  | 10       | 0.16          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 4        | 0.16          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 5        | 0.16          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 5        | 0.16          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 5        | 0.16          |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 5        | 0.16          |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 6        | 0.16          |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 2        | 0.16          |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 8        | 0.16          |
| (1,3005) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB3  | 9        | 0.16          |
| (1,2993) | 1:126:B:GLU:HB3  | 1:133:B:TYR:HB2  | 3        | 0.16          |
| (1,2980) | 1:125:B:GLU:HA   | 1:125:B:GLU:HG2  | 2        | 0.16          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 8        | 0.16          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 9        | 0.16          |
| (1,2928) | 1:120:B:ILE:HG21 | 1:122:B:GLY:HA3  | 4        | 0.16          |
| (1,2928) | 1:120:B:ILE:HG22 | 1:122:B:GLY:HA3  | 4        | 0.16          |
| (1,2928) | 1:120:B:ILE:HG23 | 1:122:B:GLY:HA3  | 4        | 0.16          |
| (1,2886) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG13 | 9        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 3        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 3        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 3        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 3        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 3        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 3        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 3        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 3        | 0.16          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 3        | 0.16          |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD21 | 4        | 0.16          |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD22 | 4        | 0.16          |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD23 | 4        | 0.16          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 9        | 0.16          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 9        | 0.16          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 9        | 0.16          |
| (1,2831) | 1:117:B:VAL:HA   | 1:148:B:VAL:HB   | 3        | 0.16          |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 1        | 0.16          |
| (1,2630) | 1:109:B:LEU:HA   | 1:109:B:LEU:HB2  | 4        | 0.16          |
| (1,2577) | 1:105:B:ALA:HB1  | 1:107:B:ASP:HB2  | 2        | 0.16          |
| (1,2577) | 1:105:B:ALA:HB2  | 1:107:B:ASP:HB2  | 2        | 0.16          |
| (1,2577) | 1:105:B:ALA:HB3  | 1:107:B:ASP:HB2  | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG11 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG12 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG13 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG11 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG12 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG13 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG11 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG12 | 2        | 0.16          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG13 | 2        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 4        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 7        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 7        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 7        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 7        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 7        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 7        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 7        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 7        | 0.16          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 7        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG21 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG22 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD11  | 1:101:B:VAL:HG23 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG21 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG22 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD12  | 1:101:B:VAL:HG23 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG21 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG22 | 9        | 0.16          |
| (1,2507) | 1:99:B:LEU:HD13  | 1:101:B:VAL:HG23 | 9        | 0.16          |
| (1,2474) | 1:98:B:SER:HB3   | 1:162:B:THR:HA   | 3        | 0.16          |
| (1,2447) | 1:97:B:VAL:HG21  | 1:118:B:VAL:HB   | 7        | 0.16          |
| (1,2447) | 1:97:B:VAL:HG22  | 1:118:B:VAL:HB   | 7        | 0.16          |
| (1,2447) | 1:97:B:VAL:HG23  | 1:118:B:VAL:HB   | 7        | 0.16          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD1  | 7        | 0.16          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD2  | 7        | 0.16          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD1  | 7        | 0.16          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD2  | 7        | 0.16          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD1  | 7        | 0.16          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD2  | 7        | 0.16          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG21 | 5        | 0.16          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG22 | 5        | 0.16          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG23 | 5        | 0.16          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG21  | 3        | 0.16          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG22  | 3        | 0.16          |
| (1,2389) | 1:96:B:ARG:HG3   | 1:97:B:VAL:HG23  | 3        | 0.16          |
| (1,2383) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HB3  | 10       | 0.16          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 5        | 0.16          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 5        | 0.16          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 5        | 0.16          |
| (1,2353) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB3  | 4        | 0.16          |
| (1,2227) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 5        | 0.16          |
| (1,2227) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 5        | 0.16          |
| (1,2227) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 5        | 0.16          |
| (1,2194) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 8        | 0.16          |
| (1,2177) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 8        | 0.16          |
| (1,2160) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 6        | 0.16          |
| (1,2160) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 9        | 0.16          |
| (1,2095) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HG2  | 5        | 0.16          |
| (1,2095) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HG2  | 5        | 0.16          |
| (1,2095) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HG2  | 5        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2062) | 1:134:B:ILE:HA   | 1:140:A:ARG:HD3  | 8        | 0.16          |
| (1,2045) | 1:133:B:TYR:HB3  | 1:141:A:LYS:HD2  | 8        | 0.16          |
| (1,2028) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 6        | 0.16          |
| (1,2028) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 9        | 0.16          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 4        | 0.16          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 8        | 0.16          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 2        | 0.16          |
| (1,1901) | 1:161:A:GLY:H    | 1:102:A:ASN:HB2  | 5        | 0.16          |
| (1,1806) | 1:152:A:GLN:HE22 | 1:149:A:ASP:HB2  | 10       | 0.16          |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 3        | 0.16          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 3        | 0.16          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 3        | 0.16          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 3        | 0.16          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD11  | 6        | 0.16          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD12  | 6        | 0.16          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD13  | 6        | 0.16          |
| (1,1668) | 1:135:A:SER:H    | 1:135:A:SER:HB3  | 3        | 0.16          |
| (1,1654) | 1:134:A:ILE:H    | 1:127:A:ARG:HB2  | 5        | 0.16          |
| (1,1647) | 1:132:A:GLY:H    | 1:131:A:HIS:HB3  | 3        | 0.16          |
| (1,1618) | 1:128:A:GLN:HE21 | 1:129:A:ASP:H    | 1        | 0.16          |
| (1,1606) | 1:128:A:GLN:H    | 1:133:A:TYR:HD1  | 8        | 0.16          |
| (1,1606) | 1:128:A:GLN:H    | 1:133:A:TYR:HD2  | 8        | 0.16          |
| (1,1588) | 1:126:A:GLU:H    | 1:125:A:GLU:HG3  | 10       | 0.16          |
| (1,1566) | 1:123:A:LYS:H    | 1:109:A:LEU:HB2  | 2        | 0.16          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG21 | 10       | 0.16          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG22 | 10       | 0.16          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG23 | 10       | 0.16          |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 9        | 0.16          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 8        | 0.16          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD21 | 2        | 0.16          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD22 | 2        | 0.16          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD23 | 2        | 0.16          |
| (1,1382) | 1:102:A:ASN:HD22 | 1:161:A:GLY:HA2  | 8        | 0.16          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG21 | 3        | 0.16          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG22 | 3        | 0.16          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG23 | 3        | 0.16          |
| (1,1333) | 1:95:A:TRP:H     | 1:166:A:GLU:HG3  | 2        | 0.16          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 7        | 0.16          |
| (1,1277) | 1:168:A:PRO:HA   | 1:169:A:MET:HG3  | 7        | 0.16          |
| (1,1197) | 1:158:A:SER:HB3  | 1:159:A:PRO:HD3  | 10       | 0.16          |
| (1,1191) | 1:158:A:SER:HB2  | 1:160:A:GLU:HG2  | 1        | 0.16          |
| (1,1181) | 1:158:A:SER:HA   | 1:158:A:SER:HB2  | 2        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 2        | 0.16          |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 2        | 0.16          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 2        | 0.16          |
| (1,1172) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB2  | 8        | 0.16          |
| (1,1172) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB2  | 8        | 0.16          |
| (1,1172) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB2  | 8        | 0.16          |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 8        | 0.16          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD21 | 2        | 0.16          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD22 | 2        | 0.16          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD23 | 2        | 0.16          |
| (1,1085) | 1:153:A:VAL:HG11 | 1:155:A:SER:HB3  | 2        | 0.16          |
| (1,1085) | 1:153:A:VAL:HG12 | 1:155:A:SER:HB3  | 2        | 0.16          |
| (1,1085) | 1:153:A:VAL:HG13 | 1:155:A:SER:HB3  | 2        | 0.16          |
| (1,1079) | 1:153:A:VAL:HB   | 1:154:A:SER:HA   | 2        | 0.16          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 2        | 0.16          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 3        | 0.16          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 4        | 0.16          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 7        | 0.16          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 8        | 0.16          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 9        | 0.16          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 10       | 0.16          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 1        | 0.16          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 3        | 0.16          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 8        | 0.16          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 9        | 0.16          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 1        | 0.16          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 1        | 0.16          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 1        | 0.16          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD11 | 8        | 0.16          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD12 | 8        | 0.16          |
| (1,896)  | 1:143:A:THR:HB   | 1:144:A:LEU:HD13 | 8        | 0.16          |
| (1,858)  | 1:141:A:LYS:HG3  | 1:141:A:LYS:HE2  | 3        | 0.16          |
| (1,856)  | 1:141:A:LYS:HG2  | 1:142:A:TYR:HB3  | 3        | 0.16          |
| (1,831)  | 1:139:A:THR:HB   | 1:141:A:LYS:HE2  | 3        | 0.16          |
| (1,779)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HE1  | 2        | 0.16          |
| (1,773)  | 1:130:A:GLU:HA   | 1:130:A:GLU:HG3  | 2        | 0.16          |
| (1,764)  | 1:129:A:ASP:HA   | 1:129:A:ASP:HB3  | 2        | 0.16          |
| (1,756)  | 1:128:A:GLN:HB3  | 1:133:A:TYR:HD1  | 8        | 0.16          |
| (1,756)  | 1:128:A:GLN:HB3  | 1:133:A:TYR:HD2  | 8        | 0.16          |
| (1,732)  | 1:126:A:GLU:HG3  | 1:134:A:ILE:HG22 | 6        | 0.16          |
| (1,723)  | 1:126:A:GLU:HG2  | 1:135:A:SER:HB2  | 6        | 0.16          |
| (1,703)  | 1:125:A:GLU:HA   | 1:135:A:SER:HB2  | 5        | 0.16          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,680) | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 9        | 0.16          |
| (1,680) | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 10       | 0.16          |
| (1,654) | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD2  | 10       | 0.16          |
| (1,654) | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD2  | 10       | 0.16          |
| (1,654) | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD2  | 10       | 0.16          |
| (1,648) | 1:120:A:ILE:HG21 | 1:139:A:THR:HA   | 10       | 0.16          |
| (1,648) | 1:120:A:ILE:HG22 | 1:139:A:THR:HA   | 10       | 0.16          |
| (1,648) | 1:120:A:ILE:HG23 | 1:139:A:THR:HA   | 10       | 0.16          |
| (1,605) | 1:119:A:GLU:HA   | 1:120:A:ILE:HG13 | 1        | 0.16          |
| (1,605) | 1:119:A:GLU:HA   | 1:120:A:ILE:HG13 | 10       | 0.16          |
| (1,559) | 1:117:A:VAL:HG11 | 1:141:A:LYS:HE3  | 4        | 0.16          |
| (1,559) | 1:117:A:VAL:HG12 | 1:141:A:LYS:HE3  | 4        | 0.16          |
| (1,559) | 1:117:A:VAL:HG13 | 1:141:A:LYS:HE3  | 4        | 0.16          |
| (1,558) | 1:117:A:VAL:HG11 | 1:141:A:LYS:HE2  | 4        | 0.16          |
| (1,558) | 1:117:A:VAL:HG12 | 1:141:A:LYS:HE2  | 4        | 0.16          |
| (1,558) | 1:117:A:VAL:HG13 | 1:141:A:LYS:HE2  | 4        | 0.16          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 7        | 0.16          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 7        | 0.16          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 7        | 0.16          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 9        | 0.16          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 9        | 0.16          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 9        | 0.16          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG21 | 4        | 0.16          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG22 | 4        | 0.16          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG23 | 4        | 0.16          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG21 | 6        | 0.16          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG22 | 6        | 0.16          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG23 | 6        | 0.16          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 2        | 0.16          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 2        | 0.16          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 2        | 0.16          |
| (1,502) | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 1        | 0.16          |
| (1,502) | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 1        | 0.16          |
| (1,502) | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 1        | 0.16          |
| (1,502) | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 8        | 0.16          |
| (1,502) | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 8        | 0.16          |
| (1,502) | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 8        | 0.16          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG21 | 3        | 0.16          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG22 | 3        | 0.16          |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG23 | 3        | 0.16          |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG21 | 3        | 0.16          |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG22 | 3        | 0.16          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG23 | 3        | 0.16          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG21 | 3        | 0.16          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG22 | 3        | 0.16          |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG23 | 3        | 0.16          |
| (1,347) | 1:108:A:GLU:HG3  | 1:123:A:LYS:HD2  | 2        | 0.16          |
| (1,337) | 1:108:A:GLU:HA   | 1:108:A:GLU:HG3  | 1        | 0.16          |
| (1,331) | 1:107:A:ASP:HA   | 1:108:A:GLU:HG2  | 1        | 0.16          |
| (1,298) | 1:105:A:ALA:HB1  | 1:108:A:GLU:HB2  | 1        | 0.16          |
| (1,298) | 1:105:A:ALA:HB2  | 1:108:A:GLU:HB2  | 1        | 0.16          |
| (1,298) | 1:105:A:ALA:HB3  | 1:108:A:GLU:HB2  | 1        | 0.16          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 6        | 0.16          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 6        | 0.16          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 6        | 0.16          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 8        | 0.16          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 8        | 0.16          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 8        | 0.16          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 4        | 0.16          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 4        | 0.16          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 4        | 0.16          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG11 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG12 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD11  | 1:111:A:VAL:HG13 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG11 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG12 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD12  | 1:111:A:VAL:HG13 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG11 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG12 | 4        | 0.16          |
| (1,229) | 1:99:A:LEU:HD13  | 1:111:A:VAL:HG13 | 4        | 0.16          |
| (1,155) | 1:97:A:VAL:HG21  | 1:144:A:LEU:HB2  | 8        | 0.16          |
| (1,155) | 1:97:A:VAL:HG22  | 1:144:A:LEU:HB2  | 8        | 0.16          |
| (1,155) | 1:97:A:VAL:HG23  | 1:144:A:LEU:HB2  | 8        | 0.16          |
| (1,154) | 1:97:A:VAL:HG21  | 1:142:A:TYR:HE1  | 8        | 0.16          |
| (1,154) | 1:97:A:VAL:HG21  | 1:142:A:TYR:HE2  | 8        | 0.16          |
| (1,154) | 1:97:A:VAL:HG22  | 1:142:A:TYR:HE1  | 8        | 0.16          |
| (1,154) | 1:97:A:VAL:HG22  | 1:142:A:TYR:HE2  | 8        | 0.16          |
| (1,154) | 1:97:A:VAL:HG23  | 1:142:A:TYR:HE1  | 8        | 0.16          |
| (1,154) | 1:97:A:VAL:HG23  | 1:142:A:TYR:HE2  | 8        | 0.16          |
| (1,132) | 1:97:A:VAL:HB    | 1:165:A:VAL:HG21 | 5        | 0.16          |
| (1,132) | 1:97:A:VAL:HB    | 1:165:A:VAL:HG22 | 5        | 0.16          |
| (1,132) | 1:97:A:VAL:HB    | 1:165:A:VAL:HG23 | 5        | 0.16          |
| (1,101) | 1:96:A:ARG:HB3   | 1:166:A:GLU:HA   | 2        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG21 | 5        | 0.16          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG22 | 5        | 0.16          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG23 | 5        | 0.16          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG21 | 4        | 0.16          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG22 | 4        | 0.16          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG23 | 4        | 0.16          |
| (1,72)   | 1:95:A:TRP:HB2   | 1:168:A:PRO:HB3  | 5        | 0.16          |
| (1,60)   | 1:95:A:TRP:HB2   | 1:95:A:TRP:HE3   | 3        | 0.16          |
| (1,4192) | 1:161:B:GLY:H    | 1:161:B:GLY:HA2  | 2        | 0.15          |
| (1,4192) | 1:161:B:GLY:H    | 1:161:B:GLY:HA2  | 7        | 0.15          |
| (1,4190) | 1:161:B:GLY:H    | 1:160:B:GLU:HB3  | 1        | 0.15          |
| (1,4128) | 1:155:B:SER:H    | 1:154:B:SER:HB2  | 5        | 0.15          |
| (1,4115) | 1:154:B:SER:H    | 1:155:B:SER:HB2  | 6        | 0.15          |
| (1,4077) | 1:152:B:GLN:HE21 | 1:149:B:ASP:HB2  | 6        | 0.15          |
| (1,4034) | 1:148:B:VAL:H    | 1:149:B:ASP:H    | 6        | 0.15          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD11 | 9        | 0.15          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD12 | 9        | 0.15          |
| (1,4007) | 1:144:B:LEU:H    | 1:144:B:LEU:HD13 | 9        | 0.15          |
| (1,3955) | 1:137:B:CYS:H    | 1:136:B:ARG:HB3  | 7        | 0.15          |
| (1,3936) | 1:134:B:ILE:H    | 1:127:B:ARG:HG2  | 4        | 0.15          |
| (1,3936) | 1:134:B:ILE:H    | 1:127:B:ARG:HG2  | 5        | 0.15          |
| (1,3918) | 1:131:B:HIS:H    | 1:130:B:GLU:HG2  | 2        | 0.15          |
| (1,3907) | 1:129:B:ASP:H    | 1:132:B:GLY:HA3  | 5        | 0.15          |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 9        | 0.15          |
| (1,3889) | 1:128:B:GLN:HE22 | 1:128:B:GLN:HB2  | 3        | 0.15          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD1  | 9        | 0.15          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD2  | 9        | 0.15          |
| (1,3826) | 1:120:B:ILE:H    | 1:140:B:ARG:HG3  | 8        | 0.15          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG21 | 10       | 0.15          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG22 | 10       | 0.15          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG23 | 10       | 0.15          |
| (1,3781) | 1:117:B:VAL:H    | 1:115:B:ASP:HB2  | 6        | 0.15          |
| (1,3739) | 1:112:B:LYS:H    | 1:112:B:LYS:HB3  | 2        | 0.15          |
| (1,3737) | 1:112:B:LYS:H    | 1:111:B:VAL:HG11 | 5        | 0.15          |
| (1,3737) | 1:112:B:LYS:H    | 1:111:B:VAL:HG12 | 5        | 0.15          |
| (1,3737) | 1:112:B:LYS:H    | 1:111:B:VAL:HG13 | 5        | 0.15          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 10       | 0.15          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 10       | 0.15          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 10       | 0.15          |
| (1,3726) | 1:111:B:VAL:H    | 1:110:B:THR:HB   | 4        | 0.15          |
| (1,3672) | 1:105:B:ALA:H    | 1:108:B:GLU:HB3  | 4        | 0.15          |
| (1,3664) | 1:102:B:ASN:HD22 | 1:161:B:GLY:HA3  | 6        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3608) | 1:94:B:ARG:H     | 1:169:B:MET:HG2  | 10       | 0.15          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG21  | 8        | 0.15          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG22  | 8        | 0.15          |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG23  | 8        | 0.15          |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 9        | 0.15          |
| (1,3557) | 1:168:B:PRO:HA   | 1:169:B:MET:HG2  | 6        | 0.15          |
| (1,3498) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HA   | 7        | 0.15          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 6        | 0.15          |
| (1,3479) | 1:159:B:PRO:HA   | 1:159:B:PRO:HB3  | 4        | 0.15          |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 6        | 0.15          |
| (1,3453) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB2  | 5        | 0.15          |
| (1,3453) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB2  | 5        | 0.15          |
| (1,3453) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB2  | 5        | 0.15          |
| (1,3444) | 1:157:B:LEU:HG   | 1:161:B:GLY:HA3  | 3        | 0.15          |
| (1,3438) | 1:157:B:LEU:HB3  | 1:157:B:LEU:HG   | 9        | 0.15          |
| (1,3430) | 1:157:B:LEU:HA   | 1:163:B:LEU:HB3  | 2        | 0.15          |
| (1,3430) | 1:157:B:LEU:HA   | 1:163:B:LEU:HB3  | 3        | 0.15          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD21 | 3        | 0.15          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD22 | 3        | 0.15          |
| (1,3421) | 1:156:B:SER:HB3  | 1:157:B:LEU:HD23 | 3        | 0.15          |
| (1,3391) | 1:155:B:SER:HA   | 1:165:B:VAL:HA   | 6        | 0.15          |
| (1,3358) | 1:153:B:VAL:HA   | 1:168:B:PRO:HD2  | 4        | 0.15          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 5        | 0.15          |
| (1,3270) | 1:148:B:VAL:HA   | 1:169:B:MET:HA   | 5        | 0.15          |
| (1,3266) | 1:148:B:VAL:HA   | 1:149:B:ASP:HB3  | 1        | 0.15          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 8        | 0.15          |
| (1,3143) | 1:141:B:LYS:HG3  | 1:142:B:TYR:HB3  | 9        | 0.15          |
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 9        | 0.15          |
| (1,3063) | 1:131:B:HIS:HB2  | 1:132:B:GLY:HA2  | 10       | 0.15          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE1  | 1        | 0.15          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE2  | 1        | 0.15          |
| (1,3018) | 1:127:B:ARG:HA   | 1:127:B:ARG:HD3  | 4        | 0.15          |
| (1,3018) | 1:127:B:ARG:HA   | 1:127:B:ARG:HD3  | 6        | 0.15          |
| (1,3005) | 1:126:B:GLU:HG2  | 1:135:B:SER:HB3  | 1        | 0.15          |
| (1,2993) | 1:126:B:GLU:HB3  | 1:133:B:TYR:HB2  | 7        | 0.15          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 4        | 0.15          |
| (1,2945) | 1:121:B:THR:HA   | 1:139:B:THR:HA   | 9        | 0.15          |
| (1,2929) | 1:120:B:ILE:HG21 | 1:139:B:THR:HA   | 4        | 0.15          |
| (1,2929) | 1:120:B:ILE:HG22 | 1:139:B:THR:HA   | 4        | 0.15          |
| (1,2929) | 1:120:B:ILE:HG23 | 1:139:B:THR:HA   | 4        | 0.15          |
| (1,2929) | 1:120:B:ILE:HG21 | 1:139:B:THR:HA   | 7        | 0.15          |
| (1,2929) | 1:120:B:ILE:HG22 | 1:139:B:THR:HA   | 7        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2929) | 1:120:B:ILE:HG23 | 1:139:B:THR:HA   | 7        | 0.15          |
| (1,2928) | 1:120:B:ILE:HG21 | 1:122:B:GLY:HA3  | 10       | 0.15          |
| (1,2928) | 1:120:B:ILE:HG22 | 1:122:B:GLY:HA3  | 10       | 0.15          |
| (1,2928) | 1:120:B:ILE:HG23 | 1:122:B:GLY:HA3  | 10       | 0.15          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD11 | 2        | 0.15          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD12 | 2        | 0.15          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD13 | 2        | 0.15          |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE1  | 10       | 0.15          |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE2  | 10       | 0.15          |
| (1,2900) | 1:119:B:GLU:HG2  | 1:141:B:LYS:HE3  | 2        | 0.15          |
| (1,2889) | 1:119:B:GLU:HA   | 1:141:B:LYS:HA   | 3        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 2        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 6        | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 10       | 0.15          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 10       | 0.15          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG11 | 4        | 0.15          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG12 | 4        | 0.15          |
| (1,2832) | 1:117:B:VAL:HA   | 1:148:B:VAL:HG13 | 4        | 0.15          |
| (1,2831) | 1:117:B:VAL:HA   | 1:148:B:VAL:HB   | 10       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 1        | 0.15          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 1        | 0.15          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 1        | 0.15          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 8        | 0.15          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 8        | 0.15          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 8        | 0.15          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG21 | 3        | 0.15          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG22 | 3        | 0.15          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG23 | 3        | 0.15          |
| (1,2738) | 1:112:B:LYS:HB2  | 1:120:B:ILE:HA   | 7        | 0.15          |
| (1,2736) | 1:112:B:LYS:HB2  | 1:112:B:LYS:HE3  | 9        | 0.15          |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE3  | 4        | 0.15          |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE3  | 4        | 0.15          |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE3  | 4        | 0.15          |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 9        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 4        | 0.15          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 4        | 0.15          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 7        | 0.15          |
| (1,2592) | 1:106:B:PRO:HA   | 1:109:B:LEU:HB2  | 1        | 0.15          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 4        | 0.15          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 4        | 0.15          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 4        | 0.15          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD11 | 6        | 0.15          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD12 | 6        | 0.15          |
| (1,2570) | 1:105:B:ALA:HA   | 1:157:B:LEU:HD13 | 6        | 0.15          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD11 | 6        | 0.15          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD12 | 6        | 0.15          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD13 | 6        | 0.15          |
| (1,2540) | 1:100:B:ASP:HA   | 1:100:B:ASP:HB3  | 9        | 0.15          |
| (1,2436) | 1:97:B:VAL:HG21  | 1:144:B:LEU:HB2  | 8        | 0.15          |
| (1,2436) | 1:97:B:VAL:HG22  | 1:144:B:LEU:HB2  | 8        | 0.15          |
| (1,2436) | 1:97:B:VAL:HG23  | 1:144:B:LEU:HB2  | 8        | 0.15          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG21  | 4        | 0.15          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG22  | 4        | 0.15          |
| (1,2389) | 1:96:B:ARG:HG2   | 1:97:B:VAL:HG23  | 4        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2361) | 1:96:B:ARG:HA    | 1:96:B:ARG:HD3   | 7        | 0.15          |
| (1,2361) | 1:96:B:ARG:HA    | 1:96:B:ARG:HD3   | 10       | 0.15          |
| (1,2355) | 1:95:B:TRP:HB3   | 1:169:B:MET:HB3  | 1        | 0.15          |
| (1,2342) | 1:95:B:TRP:HB2   | 1:96:B:ARG:HA    | 8        | 0.15          |
| (1,2318) | 1:94:B:ARG:HB2   | 1:96:B:ARG:HA    | 6        | 0.15          |
| (1,2304) | 1:94:B:ARG:HA    | 1:94:B:ARG:HB3   | 10       | 0.15          |
| (1,2225) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 2        | 0.15          |
| (1,2225) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 2        | 0.15          |
| (1,2225) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 2        | 0.15          |
| (1,2225) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 8        | 0.15          |
| (1,2225) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 8        | 0.15          |
| (1,2225) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 8        | 0.15          |
| (1,2160) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 1        | 0.15          |
| (1,2093) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 2        | 0.15          |
| (1,2093) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 2        | 0.15          |
| (1,2093) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 2        | 0.15          |
| (1,2093) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 8        | 0.15          |
| (1,2093) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 8        | 0.15          |
| (1,2093) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 8        | 0.15          |
| (1,2028) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB3  | 1        | 0.15          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 10       | 0.15          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG11 | 9        | 0.15          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG12 | 9        | 0.15          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG13 | 9        | 0.15          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG21 | 6        | 0.15          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG22 | 6        | 0.15          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG23 | 6        | 0.15          |
| (1,1901) | 1:161:A:GLY:H    | 1:102:A:ASN:HB2  | 4        | 0.15          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG21 | 10       | 0.15          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG22 | 10       | 0.15          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG23 | 10       | 0.15          |
| (1,1816) | 1:153:A:VAL:H    | 1:149:A:ASP:HB2  | 4        | 0.15          |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 4        | 0.15          |
| (1,1743) | 1:148:A:VAL:H    | 1:146:A:PRO:HB3  | 5        | 0.15          |
| (1,1733) | 1:147:A:GLY:H    | 1:146:A:PRO:HG2  | 8        | 0.15          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 5        | 0.15          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 5        | 0.15          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 5        | 0.15          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 10       | 0.15          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 10       | 0.15          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 10       | 0.15          |
| (1,1703) | 1:142:A:TYR:H    | 1:141:A:LYS:HG2  | 9        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD21  | 2        | 0.15          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD22  | 2        | 0.15          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD23  | 2        | 0.15          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD21  | 10       | 0.15          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD22  | 10       | 0.15          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD23  | 10       | 0.15          |
| (1,1667) | 1:135:A:SER:H    | 1:135:A:SER:HB2  | 9        | 0.15          |
| (1,1647) | 1:132:A:GLY:H    | 1:131:A:HIS:HB3  | 7        | 0.15          |
| (1,1642) | 1:132:A:GLY:H    | 1:129:A:ASP:HB2  | 4        | 0.15          |
| (1,1626) | 1:129:A:ASP:H    | 1:132:A:GLY:HA3  | 3        | 0.15          |
| (1,1622) | 1:129:A:ASP:H    | 1:129:A:ASP:HB3  | 9        | 0.15          |
| (1,1611) | 1:128:A:GLN:HE22 | 1:128:A:GLN:H    | 2        | 0.15          |
| (1,1600) | 1:128:A:GLN:H    | 1:127:A:ARG:HD2  | 1        | 0.15          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB1  | 7        | 0.15          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB2  | 7        | 0.15          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB3  | 7        | 0.15          |
| (1,1546) | 1:120:A:ILE:H    | 1:142:A:TYR:H    | 4        | 0.15          |
| (1,1517) | 1:118:A:VAL:H    | 1:142:A:TYR:HB2  | 5        | 0.15          |
| (1,1509) | 1:117:A:VAL:H    | 1:144:A:LEU:H    | 5        | 0.15          |
| (1,1489) | 1:114:A:LYS:H    | 1:119:A:GLU:H    | 2        | 0.15          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD11 | 3        | 0.15          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD12 | 3        | 0.15          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD13 | 3        | 0.15          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD11 | 5        | 0.15          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD12 | 5        | 0.15          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD13 | 5        | 0.15          |
| (1,1389) | 1:105:A:ALA:H    | 1:106:A:PRO:HD3  | 10       | 0.15          |
| (1,1373) | 1:102:A:ASN:HD21 | 1:161:A:GLY:HA2  | 2        | 0.15          |
| (1,1345) | 1:97:A:VAL:H     | 1:165:A:VAL:H    | 7        | 0.15          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 6        | 0.15          |
| (1,1210) | 1:160:A:GLU:HB2  | 1:162:A:THR:HB   | 6        | 0.15          |
| (1,1197) | 1:158:A:SER:HB3  | 1:159:A:PRO:HD3  | 3        | 0.15          |
| (1,1189) | 1:158:A:SER:HA   | 1:160:A:GLU:HB3  | 5        | 0.15          |
| (1,1177) | 1:157:A:LEU:HD21 | 1:161:A:GLY:HA3  | 4        | 0.15          |
| (1,1177) | 1:157:A:LEU:HD22 | 1:161:A:GLY:HA3  | 4        | 0.15          |
| (1,1177) | 1:157:A:LEU:HD23 | 1:161:A:GLY:HA3  | 4        | 0.15          |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 3        | 0.15          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 8        | 0.15          |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 4        | 0.15          |
| (1,1148) | 1:157:A:LEU:HA   | 1:162:A:THR:HB   | 2        | 0.15          |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 4        | 0.15          |
| (1,1119) | 1:155:A:SER:HB2  | 1:165:A:VAL:HA   | 6        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1110) | 1:155:A:SER:HA   | 1:165:A:VAL:HA   | 10       | 0.15          |
| (1,1035) | 1:150:A:PRO:HA   | 1:150:A:PRO:HB3  | 6        | 0.15          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 5        | 0.15          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 10       | 0.15          |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 3        | 0.15          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 5        | 0.15          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 5        | 0.15          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 5        | 0.15          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG11 | 9        | 0.15          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG12 | 9        | 0.15          |
| (1,882)  | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG13 | 9        | 0.15          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG11 | 9        | 0.15          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG12 | 9        | 0.15          |
| (1,882)  | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG13 | 9        | 0.15          |
| (1,862)  | 1:141:A:LYS:HG3  | 1:142:A:TYR:HB3  | 6        | 0.15          |
| (1,845)  | 1:141:A:LYS:HA   | 1:141:A:LYS:HD3  | 1        | 0.15          |
| (1,816)  | 1:137:A:CYS:HA   | 1:138:A:PHE:HD1  | 8        | 0.15          |
| (1,816)  | 1:137:A:CYS:HA   | 1:138:A:PHE:HD2  | 8        | 0.15          |
| (1,779)  | 1:131:A:HIS:HA   | 1:131:A:HIS:HE1  | 3        | 0.15          |
| (1,772)  | 1:130:A:GLU:HA   | 1:130:A:GLU:HG2  | 4        | 0.15          |
| (1,734)  | 1:127:A:ARG:HA   | 1:127:A:ARG:HB3  | 2        | 0.15          |
| (1,717)  | 1:126:A:GLU:HG2  | 1:127:A:ARG:HG3  | 9        | 0.15          |
| (1,700)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG3  | 5        | 0.15          |
| (1,699)  | 1:125:A:GLU:HA   | 1:125:A:GLU:HG2  | 8        | 0.15          |
| (1,680)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 6        | 0.15          |
| (1,664)  | 1:121:A:THR:HA   | 1:139:A:THR:HA   | 5        | 0.15          |
| (1,664)  | 1:121:A:THR:HA   | 1:139:A:THR:HA   | 7        | 0.15          |
| (1,652)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HB2  | 6        | 0.15          |
| (1,652)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HB2  | 6        | 0.15          |
| (1,652)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HB2  | 6        | 0.15          |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD11 | 4        | 0.15          |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD12 | 4        | 0.15          |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD13 | 4        | 0.15          |
| (1,639)  | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 9        | 0.15          |
| (1,637)  | 1:120:A:ILE:HB   | 1:142:A:TYR:HE1  | 10       | 0.15          |
| (1,637)  | 1:120:A:ILE:HB   | 1:142:A:TYR:HE2  | 10       | 0.15          |
| (1,610)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HD3  | 9        | 0.15          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 7        | 0.15          |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 7        | 0.15          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 7        | 0.15          |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 7        | 0.15          |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 7        | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 7        | 0.15          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD21 | 6        | 0.15          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD22 | 6        | 0.15          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD23 | 6        | 0.15          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG21 | 9        | 0.15          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG22 | 9        | 0.15          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG23 | 9        | 0.15          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 6        | 0.15          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 6        | 0.15          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 6        | 0.15          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG21 | 1        | 0.15          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG22 | 1        | 0.15          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG23 | 1        | 0.15          |
| (1,383) | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 6        | 0.15          |
| (1,383) | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 6        | 0.15          |
| (1,383) | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 6        | 0.15          |
| (1,383) | 1:109:A:LEU:HD21 | 1:122:A:GLY:HA3  | 10       | 0.15          |
| (1,383) | 1:109:A:LEU:HD22 | 1:122:A:GLY:HA3  | 10       | 0.15          |
| (1,383) | 1:109:A:LEU:HD23 | 1:122:A:GLY:HA3  | 10       | 0.15          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 7        | 0.15          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 7        | 0.15          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD11 | 8        | 0.15          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD12 | 8        | 0.15          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD13 | 8        | 0.15          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD21 | 4        | 0.15          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD22 | 4        | 0.15          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD23 | 4        | 0.15          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD21 | 6        | 0.15          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD22 | 6        | 0.15          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD23 | 6        | 0.15          |
| (1,298) | 1:105:A:ALA:HB1  | 1:108:A:GLU:HB2  | 6        | 0.15          |
| (1,298) | 1:105:A:ALA:HB2  | 1:108:A:GLU:HB2  | 6        | 0.15          |
| (1,298) | 1:105:A:ALA:HB3  | 1:108:A:GLU:HB2  | 6        | 0.15          |
| (1,206) | 1:99:A:LEU:HA    | 1:120:A:ILE:HD11 | 2        | 0.15          |
| (1,206) | 1:99:A:LEU:HA    | 1:120:A:ILE:HD12 | 2        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,206)  | 1:99:A:LEU:HA    | 1:120:A:ILE:HD13 | 2        | 0.15          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG21 | 2        | 0.15          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG22 | 2        | 0.15          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG23 | 2        | 0.15          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG21 | 7        | 0.15          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG22 | 7        | 0.15          |
| (1,88)   | 1:96:A:ARG:HA    | 1:165:A:VAL:HG23 | 7        | 0.15          |
| (1,80)   | 1:96:A:ARG:HA    | 1:96:A:ARG:HD3   | 9        | 0.15          |
| (1,76)   | 1:95:A:TRP:HE3   | 1:166:A:GLU:HA   | 10       | 0.15          |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 1        | 0.15          |
| (1,4280) | 1:169:B:MET:H    | 1:169:B:MET:HB3  | 6        | 0.14          |
| (1,4278) | 1:169:B:MET:H    | 1:169:B:MET:HA   | 4        | 0.14          |
| (1,4262) | 1:167:B:ALA:H    | 1:166:B:GLU:HB2  | 1        | 0.14          |
| (1,4239) | 1:165:B:VAL:H    | 1:166:B:GLU:HB3  | 10       | 0.14          |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD11 | 9        | 0.14          |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD12 | 9        | 0.14          |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD13 | 9        | 0.14          |
| (1,4192) | 1:161:B:GLY:H    | 1:161:B:GLY:HA2  | 6        | 0.14          |
| (1,4183) | 1:161:B:GLY:H    | 1:102:B:ASN:HB3  | 9        | 0.14          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG21 | 3        | 0.14          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG22 | 3        | 0.14          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG23 | 3        | 0.14          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG21 | 5        | 0.14          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG22 | 5        | 0.14          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG23 | 5        | 0.14          |
| (1,4089) | 1:152:B:GLN:HE22 | 1:152:B:GLN:HB2  | 4        | 0.14          |
| (1,4085) | 1:152:B:GLN:HE21 | 1:169:B:MET:HA   | 10       | 0.14          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 5        | 0.14          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 5        | 0.14          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 5        | 0.14          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 6        | 0.14          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 6        | 0.14          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 6        | 0.14          |
| (1,4075) | 1:152:B:GLN:H    | 1:168:B:PRO:HD3  | 5        | 0.14          |
| (1,4033) | 1:148:B:VAL:H    | 1:149:B:ASP:HB2  | 1        | 0.14          |
| (1,4014) | 1:147:B:GLY:H    | 1:146:B:PRO:HG2  | 9        | 0.14          |
| (1,3936) | 1:134:B:ILE:H    | 1:127:B:ARG:HG2  | 1        | 0.14          |
| (1,3915) | 1:131:B:HIS:H    | 1:129:B:ASP:HB3  | 3        | 0.14          |
| (1,3910) | 1:129:B:ASP:H    | 1:133:B:TYR:HB2  | 2        | 0.14          |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 3        | 0.14          |
| (1,3879) | 1:128:B:GLN:H    | 1:127:B:ARG:HG2  | 3        | 0.14          |
| (1,3869) | 1:126:B:GLU:H    | 1:125:B:GLU:HG3  | 8        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG21 | 1        | 0.14          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG22 | 1        | 0.14          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG23 | 1        | 0.14          |
| (1,3759) | 1:114:B:LYS:H    | 1:112:B:LYS:HD3  | 1        | 0.14          |
| (1,3733) | 1:112:B:LYS:H    | 1:99:B:LEU:HD21  | 2        | 0.14          |
| (1,3733) | 1:112:B:LYS:H    | 1:99:B:LEU:HD22  | 2        | 0.14          |
| (1,3733) | 1:112:B:LYS:H    | 1:99:B:LEU:HD23  | 2        | 0.14          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD11 | 9        | 0.14          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD12 | 9        | 0.14          |
| (1,3730) | 1:111:B:VAL:H    | 1:120:B:ILE:HD13 | 9        | 0.14          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD11 | 2        | 0.14          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD12 | 2        | 0.14          |
| (1,3666) | 1:103:B:HIS:H    | 1:157:B:LEU:HD13 | 2        | 0.14          |
| (1,3654) | 1:102:B:ASN:HD21 | 1:161:B:GLY:HA2  | 8        | 0.14          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG21 | 4        | 0.14          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG22 | 4        | 0.14          |
| (1,3638) | 1:99:B:LEU:H     | 1:101:B:VAL:HG23 | 4        | 0.14          |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 5        | 0.14          |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 8        | 0.14          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 2        | 0.14          |
| (1,3453) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB2  | 8        | 0.14          |
| (1,3453) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB2  | 8        | 0.14          |
| (1,3453) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB2  | 8        | 0.14          |
| (1,3449) | 1:157:B:LEU:HD11 | 1:161:B:GLY:HA3  | 9        | 0.14          |
| (1,3449) | 1:157:B:LEU:HD12 | 1:161:B:GLY:HA3  | 9        | 0.14          |
| (1,3449) | 1:157:B:LEU:HD13 | 1:161:B:GLY:HA3  | 9        | 0.14          |
| (1,3438) | 1:157:B:LEU:HB3  | 1:157:B:LEU:HG   | 6        | 0.14          |
| (1,3360) | 1:153:B:VAL:HB   | 1:154:B:SER:HA   | 10       | 0.14          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG21 | 2        | 0.14          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG22 | 2        | 0.14          |
| (1,3317) | 1:150:B:PRO:HA   | 1:151:B:THR:HG23 | 2        | 0.14          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 1        | 0.14          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 3        | 0.14          |
| (1,3316) | 1:150:B:PRO:HA   | 1:150:B:PRO:HB3  | 7        | 0.14          |
| (1,3301) | 1:148:B:VAL:HG21 | 1:169:B:MET:HB2  | 2        | 0.14          |
| (1,3301) | 1:148:B:VAL:HG22 | 1:169:B:MET:HB2  | 2        | 0.14          |
| (1,3301) | 1:148:B:VAL:HG23 | 1:169:B:MET:HB2  | 2        | 0.14          |
| (1,3278) | 1:148:B:VAL:HB   | 1:150:B:PRO:HA   | 4        | 0.14          |
| (1,3274) | 1:148:B:VAL:HA   | 1:170:B:PRO:HG2  | 7        | 0.14          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 7        | 0.14          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 7        | 0.14          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 7        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3123) | 1:141:B:LYS:HA   | 1:141:B:LYS:HB2  | 10       | 0.14          |
| (1,3086) | 1:134:B:ILE:HG23 | 1:135:B:SER:HB2  | 9        | 0.14          |
| (1,3024) | 1:127:B:ARG:HB3  | 1:127:B:ARG:HD2  | 9        | 0.14          |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD11 | 3        | 0.14          |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD12 | 3        | 0.14          |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD13 | 3        | 0.14          |
| (1,2989) | 1:126:B:GLU:HA   | 1:134:B:ILE:HG21 | 7        | 0.14          |
| (1,2989) | 1:126:B:GLU:HA   | 1:134:B:ILE:HG22 | 7        | 0.14          |
| (1,2989) | 1:126:B:GLU:HA   | 1:134:B:ILE:HG23 | 7        | 0.14          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD11 | 6        | 0.14          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD12 | 6        | 0.14          |
| (1,2921) | 1:120:B:ILE:HG12 | 1:163:B:LEU:HD13 | 6        | 0.14          |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE1  | 1        | 0.14          |
| (1,2918) | 1:120:B:ILE:HB   | 1:142:B:TYR:HE2  | 1        | 0.14          |
| (1,2883) | 1:119:B:GLU:HA   | 1:119:B:GLU:HG3  | 8        | 0.14          |
| (1,2883) | 1:119:B:GLU:HA   | 1:119:B:GLU:HG3  | 10       | 0.14          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG21 | 2        | 0.14          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG22 | 2        | 0.14          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG23 | 2        | 0.14          |
| (1,2799) | 1:115:B:ASP:HB3  | 1:150:B:PRO:HG3  | 2        | 0.14          |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG21 | 3        | 0.14          |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG22 | 3        | 0.14          |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG23 | 3        | 0.14          |
| (1,2753) | 1:112:B:LYS:HD2  | 1:120:B:ILE:HA   | 10       | 0.14          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE3  | 2        | 0.14          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE3  | 4        | 0.14          |
| (1,2716) | 1:111:B:VAL:HG11 | 1:120:B:ILE:HG13 | 4        | 0.14          |
| (1,2716) | 1:111:B:VAL:HG12 | 1:120:B:ILE:HG13 | 4        | 0.14          |
| (1,2716) | 1:111:B:VAL:HG13 | 1:120:B:ILE:HG13 | 4        | 0.14          |
| (1,2704) | 1:111:B:VAL:HB   | 1:112:B:LYS:HA   | 5        | 0.14          |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 8        | 0.14          |
| (1,2685) | 1:110:B:THR:HG21 | 1:112:B:LYS:HB2  | 1        | 0.14          |
| (1,2685) | 1:110:B:THR:HG22 | 1:112:B:LYS:HB2  | 1        | 0.14          |
| (1,2685) | 1:110:B:THR:HG23 | 1:112:B:LYS:HB2  | 1        | 0.14          |
| (1,2654) | 1:109:B:LEU:HD11 | 1:161:B:GLY:HA3  | 4        | 0.14          |
| (1,2654) | 1:109:B:LEU:HD12 | 1:161:B:GLY:HA3  | 4        | 0.14          |
| (1,2654) | 1:109:B:LEU:HD13 | 1:161:B:GLY:HA3  | 4        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 3        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 3        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 3        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 3        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 3        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 3        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 3        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 3        | 0.14          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 3        | 0.14          |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 8        | 0.14          |
| (1,2561) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA3  | 10       | 0.14          |
| (1,2560) | 1:102:B:ASN:HB3  | 1:161:B:GLY:HA2  | 2        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD11 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD12 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG21 | 1:120:B:ILE:HD13 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD11 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD12 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG22 | 1:120:B:ILE:HD13 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD11 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD12 | 8        | 0.14          |
| (1,2553) | 1:101:B:VAL:HG23 | 1:120:B:ILE:HD13 | 8        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG11 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG12 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HG13 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG11 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG12 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HG13 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG11 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG12 | 1        | 0.14          |
| (1,2510) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HG13 | 1        | 0.14          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD11 | 4        | 0.14          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD12 | 4        | 0.14          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD13 | 4        | 0.14          |
| (1,2432) | 1:97:B:VAL:HG21  | 1:142:B:TYR:HB2  | 5        | 0.14          |
| (1,2432) | 1:97:B:VAL:HG22  | 1:142:B:TYR:HB2  | 5        | 0.14          |
| (1,2432) | 1:97:B:VAL:HG23  | 1:142:B:TYR:HB2  | 5        | 0.14          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD1  | 9        | 0.14          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD2  | 9        | 0.14          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD1  | 9        | 0.14          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD2  | 9        | 0.14          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD1  | 9        | 0.14          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD2  | 9        | 0.14          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG11 | 4        | 0.14          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG12 | 4        | 0.14          |
| (1,2410) | 1:97:B:VAL:HB    | 1:148:B:VAL:HG13 | 4        | 0.14          |
| (1,2380) | 1:96:B:ARG:HB3   | 1:164:B:THR:HB   | 1        | 0.14          |
| (1,2357) | 1:95:B:TRP:HE3   | 1:166:B:GLU:HA   | 7        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2326) | 1:94:B:ARG:HG2  | 1:168:B:PRO:HB2  | 1        | 0.14          |
| (1,2310) | 1:94:B:ARG:HA   | 1:168:B:PRO:HA   | 1        | 0.14          |
| (1,2284) | 1:89:B:ARG:HB2  | 1:90:B:HIS:HB2   | 4        | 0.14          |
| (1,2170) | 1:132:A:GLY:HA3 | 1:142:B:TYR:HA   | 5        | 0.14          |
| (1,2038) | 1:132:A:GLY:HA3 | 1:142:B:TYR:HA   | 5        | 0.14          |
| (1,1925) | 1:162:A:THR:H   | 1:160:A:GLU:HG3  | 5        | 0.14          |
| (1,1911) | 1:161:A:GLY:H   | 1:161:A:GLY:HA2  | 7        | 0.14          |
| (1,1911) | 1:161:A:GLY:H   | 1:161:A:GLY:HA2  | 10       | 0.14          |
| (1,1887) | 1:158:A:SER:H   | 1:162:A:THR:HG21 | 4        | 0.14          |
| (1,1887) | 1:158:A:SER:H   | 1:162:A:THR:HG22 | 4        | 0.14          |
| (1,1887) | 1:158:A:SER:H   | 1:162:A:THR:HG23 | 4        | 0.14          |
| (1,1877) | 1:158:A:SER:H   | 1:109:A:LEU:HD11 | 2        | 0.14          |
| (1,1877) | 1:158:A:SER:H   | 1:109:A:LEU:HD12 | 2        | 0.14          |
| (1,1877) | 1:158:A:SER:H   | 1:109:A:LEU:HD13 | 2        | 0.14          |
| (1,1870) | 1:157:A:LEU:H   | 1:157:A:LEU:HB3  | 5        | 0.14          |
| (1,1847) | 1:155:A:SER:H   | 1:154:A:SER:HB2  | 3        | 0.14          |
| (1,1834) | 1:154:A:SER:H   | 1:155:A:SER:HB2  | 6        | 0.14          |
| (1,1771) | 1:151:A:THR:H   | 1:149:A:ASP:HB3  | 6        | 0.14          |
| (1,1762) | 1:149:A:ASP:H   | 1:152:A:GLN:HB2  | 6        | 0.14          |
| (1,1743) | 1:148:A:VAL:H   | 1:146:A:PRO:HB3  | 9        | 0.14          |
| (1,1730) | 1:144:A:LEU:H   | 1:148:A:VAL:HG11 | 9        | 0.14          |
| (1,1730) | 1:144:A:LEU:H   | 1:148:A:VAL:HG12 | 9        | 0.14          |
| (1,1730) | 1:144:A:LEU:H   | 1:148:A:VAL:HG13 | 9        | 0.14          |
| (1,1703) | 1:142:A:TYR:H   | 1:141:A:LYS:HG3  | 6        | 0.14          |
| (1,1669) | 1:136:A:ARG:H   | 1:134:A:ILE:HG21 | 1        | 0.14          |
| (1,1669) | 1:136:A:ARG:H   | 1:134:A:ILE:HG22 | 1        | 0.14          |
| (1,1669) | 1:136:A:ARG:H   | 1:134:A:ILE:HG23 | 1        | 0.14          |
| (1,1657) | 1:134:A:ILE:H   | 1:133:A:TYR:HB3  | 1        | 0.14          |
| (1,1657) | 1:134:A:ILE:H   | 1:133:A:TYR:HB3  | 2        | 0.14          |
| (1,1657) | 1:134:A:ILE:H   | 1:133:A:TYR:HB3  | 3        | 0.14          |
| (1,1657) | 1:134:A:ILE:H   | 1:133:A:TYR:HB3  | 5        | 0.14          |
| (1,1651) | 1:132:A:GLY:H   | 1:133:A:TYR:HE1  | 9        | 0.14          |
| (1,1651) | 1:132:A:GLY:H   | 1:133:A:TYR:HE2  | 9        | 0.14          |
| (1,1606) | 1:128:A:GLN:H   | 1:133:A:TYR:HD1  | 3        | 0.14          |
| (1,1606) | 1:128:A:GLN:H   | 1:133:A:TYR:HD2  | 3        | 0.14          |
| (1,1581) | 1:125:A:GLU:H   | 1:108:A:GLU:HG3  | 2        | 0.14          |
| (1,1568) | 1:123:A:LYS:H   | 1:109:A:LEU:HD11 | 3        | 0.14          |
| (1,1568) | 1:123:A:LYS:H   | 1:109:A:LEU:HD12 | 3        | 0.14          |
| (1,1568) | 1:123:A:LYS:H   | 1:109:A:LEU:HD13 | 3        | 0.14          |
| (1,1566) | 1:123:A:LYS:H   | 1:109:A:LEU:HB2  | 1        | 0.14          |
| (1,1525) | 1:119:A:GLU:H   | 1:114:A:LYS:HB3  | 1        | 0.14          |
| (1,1506) | 1:117:A:VAL:H   | 1:118:A:VAL:HG21 | 3        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG22 | 3        | 0.14          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG23 | 3        | 0.14          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG21 | 8        | 0.14          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG22 | 8        | 0.14          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG23 | 8        | 0.14          |
| (1,1428) | 1:109:A:LEU:H    | 1:109:A:LEU:HB3  | 7        | 0.14          |
| (1,1400) | 1:107:A:ASP:H    | 1:106:A:PRO:HB3  | 7        | 0.14          |
| (1,1391) | 1:105:A:ALA:H    | 1:108:A:GLU:HB3  | 3        | 0.14          |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD11 | 6        | 0.14          |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD12 | 6        | 0.14          |
| (1,1385) | 1:103:A:HIS:H    | 1:157:A:LEU:HD13 | 6        | 0.14          |
| (1,1383) | 1:102:A:ASN:HD22 | 1:161:A:GLY:HA3  | 7        | 0.14          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD11 | 2        | 0.14          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD12 | 2        | 0.14          |
| (1,1371) | 1:102:A:ASN:HD21 | 1:157:A:LEU:HD13 | 2        | 0.14          |
| (1,1318) | 1:171:A:LYS:HA   | 1:171:A:LYS:HD2  | 6        | 0.14          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 8        | 0.14          |
| (1,1282) | 1:168:A:PRO:HB3  | 1:169:A:MET:HA   | 3        | 0.14          |
| (1,1174) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HG   | 10       | 0.14          |
| (1,1174) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HG   | 10       | 0.14          |
| (1,1174) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HG   | 10       | 0.14          |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 1        | 0.14          |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 2        | 0.14          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD11 | 10       | 0.14          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD12 | 10       | 0.14          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD13 | 10       | 0.14          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD21 | 8        | 0.14          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD22 | 8        | 0.14          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD23 | 8        | 0.14          |
| (1,1110) | 1:155:A:SER:HA   | 1:165:A:VAL:HA   | 7        | 0.14          |
| (1,1110) | 1:155:A:SER:HA   | 1:165:A:VAL:HA   | 9        | 0.14          |
| (1,1098) | 1:154:A:SER:HB3  | 1:166:A:GLU:HG3  | 8        | 0.14          |
| (1,1079) | 1:153:A:VAL:HB   | 1:154:A:SER:HA   | 3        | 0.14          |
| (1,1065) | 1:152:A:GLN:HB2  | 1:169:A:MET:HA   | 2        | 0.14          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 3        | 0.14          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 9        | 0.14          |
| (1,992)  | 1:148:A:VAL:HA   | 1:170:A:PRO:HB3  | 1        | 0.14          |
| (1,977)  | 1:147:A:GLY:HA3  | 1:148:A:VAL:HB   | 5        | 0.14          |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 2        | 0.14          |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG2  | 5        | 0.14          |
| (1,962)  | 1:145:A:PRO:HD2  | 1:146:A:PRO:HG3  | 10       | 0.14          |
| (1,917)  | 1:144:A:LEU:HB3  | 1:147:A:GLY:HA2  | 9        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 1        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 1        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 1        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 2        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 2        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 2        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 3        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 3        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 3        | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 10       | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 10       | 0.14          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 10       | 0.14          |
| (1,883) | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG21 | 9        | 0.14          |
| (1,883) | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG22 | 9        | 0.14          |
| (1,883) | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG23 | 9        | 0.14          |
| (1,883) | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG21 | 9        | 0.14          |
| (1,883) | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG22 | 9        | 0.14          |
| (1,883) | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG23 | 9        | 0.14          |
| (1,857) | 1:141:A:LYS:HG2  | 1:143:A:THR:HA   | 4        | 0.14          |
| (1,857) | 1:141:A:LYS:HG2  | 1:143:A:THR:HA   | 6        | 0.14          |
| (1,853) | 1:141:A:LYS:HG2  | 1:141:A:LYS:HE3  | 5        | 0.14          |
| (1,842) | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 10       | 0.14          |
| (1,831) | 1:139:A:THR:HB   | 1:141:A:LYS:HE2  | 7        | 0.14          |
| (1,805) | 1:134:A:ILE:HG21 | 1:135:A:SER:HB2  | 6        | 0.14          |
| (1,766) | 1:129:A:ASP:HA   | 1:130:A:GLU:HB2  | 1        | 0.14          |
| (1,759) | 1:128:A:GLN:HG2  | 1:133:A:TYR:HA   | 5        | 0.14          |
| (1,751) | 1:128:A:GLN:HA   | 1:134:A:ILE:HD11 | 4        | 0.14          |
| (1,751) | 1:128:A:GLN:HA   | 1:134:A:ILE:HD12 | 4        | 0.14          |
| (1,751) | 1:128:A:GLN:HA   | 1:134:A:ILE:HD13 | 4        | 0.14          |
| (1,690) | 1:123:A:LYS:HB3  | 1:137:A:CYS:HB2  | 1        | 0.14          |
| (1,684) | 1:123:A:LYS:HA   | 1:135:A:SER:HB3  | 1        | 0.14          |
| (1,652) | 1:120:A:ILE:HD11 | 1:140:A:ARG:HB2  | 8        | 0.14          |
| (1,652) | 1:120:A:ILE:HD12 | 1:140:A:ARG:HB2  | 8        | 0.14          |
| (1,652) | 1:120:A:ILE:HD13 | 1:140:A:ARG:HB2  | 8        | 0.14          |
| (1,650) | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD1  | 1        | 0.14          |
| (1,650) | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD2  | 1        | 0.14          |
| (1,650) | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD1  | 1        | 0.14          |
| (1,650) | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD2  | 1        | 0.14          |
| (1,650) | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD1  | 1        | 0.14          |
| (1,650) | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD2  | 1        | 0.14          |
| (1,640) | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD11 | 6        | 0.14          |
| (1,640) | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD12 | 6        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,640) | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD13 | 6        | 0.14          |
| (1,605) | 1:119:A:GLU:HA   | 1:120:A:ILE:HG13 | 3        | 0.14          |
| (1,604) | 1:119:A:GLU:HA   | 1:120:A:ILE:HG12 | 6        | 0.14          |
| (1,590) | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG11 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG12 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG13 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG11 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG12 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG13 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG11 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG12 | 2        | 0.14          |
| (1,590) | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG13 | 2        | 0.14          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 3        | 0.14          |
| (1,585) | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 3        | 0.14          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 3        | 0.14          |
| (1,585) | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 3        | 0.14          |
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 3        | 0.14          |
| (1,585) | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 3        | 0.14          |
| (1,571) | 1:118:A:VAL:HB   | 1:142:A:TYR:HD1  | 10       | 0.14          |
| (1,571) | 1:118:A:VAL:HB   | 1:142:A:TYR:HD2  | 10       | 0.14          |
| (1,562) | 1:117:A:VAL:HG11 | 1:142:A:TYR:HB3  | 4        | 0.14          |
| (1,562) | 1:117:A:VAL:HG12 | 1:142:A:TYR:HB3  | 4        | 0.14          |
| (1,562) | 1:117:A:VAL:HG13 | 1:142:A:TYR:HB3  | 4        | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 5        | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 5        | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 5        | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 8        | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 8        | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 8        | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 10       | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 10       | 0.14          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 10       | 0.14          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG11 | 10       | 0.14          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG12 | 10       | 0.14          |
| (1,529) | 1:116:A:GLY:HA2  | 1:148:A:VAL:HG13 | 10       | 0.14          |
| (1,509) | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 7        | 0.14          |
| (1,463) | 1:112:A:LYS:HG2  | 1:112:A:LYS:HE3  | 1        | 0.14          |
| (1,453) | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 10       | 0.14          |
| (1,418) | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 1        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 1        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 4        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 5        | 0.14          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 5        | 0.14          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD21 | 9        | 0.14          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD22 | 9        | 0.14          |
| (1,335) | 1:107:A:ASP:HA   | 1:157:A:LEU:HD23 | 9        | 0.14          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 9        | 0.14          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 9        | 0.14          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 9        | 0.14          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 10       | 0.14          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 10       | 0.14          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 10       | 0.14          |
| (1,265) | 1:100:A:ASP:HB3  | 1:162:A:THR:HA   | 9        | 0.14          |
| (1,264) | 1:100:A:ASP:HB2  | 1:162:A:THR:HB   | 4        | 0.14          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG11 | 5        | 0.14          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG12 | 5        | 0.14          |
| (1,240) | 1:99:A:LEU:HD21  | 1:111:A:VAL:HG13 | 5        | 0.14          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG11 | 5        | 0.14          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG12 | 5        | 0.14          |
| (1,240) | 1:99:A:LEU:HD22  | 1:111:A:VAL:HG13 | 5        | 0.14          |
| (1,240) | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG11 | 5        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG12 | 5        | 0.14          |
| (1,240)  | 1:99:A:LEU:HD23  | 1:111:A:VAL:HG13 | 5        | 0.14          |
| (1,236)  | 1:99:A:LEU:HD11  | 1:164:A:THR:HA   | 8        | 0.14          |
| (1,236)  | 1:99:A:LEU:HD12  | 1:164:A:THR:HA   | 8        | 0.14          |
| (1,236)  | 1:99:A:LEU:HD13  | 1:164:A:THR:HA   | 8        | 0.14          |
| (1,203)  | 1:99:A:LEU:HA    | 1:100:A:ASP:HB3  | 7        | 0.14          |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD21  | 9        | 0.14          |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD22  | 9        | 0.14          |
| (1,201)  | 1:99:A:LEU:HA    | 1:99:A:LEU:HD23  | 9        | 0.14          |
| (1,161)  | 1:97:A:VAL:HG21  | 1:166:A:GLU:HA   | 5        | 0.14          |
| (1,161)  | 1:97:A:VAL:HG22  | 1:166:A:GLU:HA   | 5        | 0.14          |
| (1,161)  | 1:97:A:VAL:HG23  | 1:166:A:GLU:HA   | 5        | 0.14          |
| (1,143)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE1  | 7        | 0.14          |
| (1,143)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE2  | 7        | 0.14          |
| (1,143)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE1  | 7        | 0.14          |
| (1,143)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE2  | 7        | 0.14          |
| (1,143)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE1  | 7        | 0.14          |
| (1,143)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE2  | 7        | 0.14          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG21 | 6        | 0.14          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG22 | 6        | 0.14          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG23 | 6        | 0.14          |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG21  | 10       | 0.14          |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG22  | 10       | 0.14          |
| (1,108)  | 1:96:A:ARG:HG2   | 1:97:A:VAL:HG23  | 10       | 0.14          |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 3        | 0.14          |
| (1,23)   | 1:94:A:ARG:HA    | 1:94:A:ARG:HB3   | 7        | 0.14          |
| (1,4220) | 1:164:B:THR:H    | 1:162:B:THR:HA   | 9        | 0.13          |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD11 | 5        | 0.13          |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD12 | 5        | 0.13          |
| (1,4219) | 1:164:B:THR:H    | 1:157:B:LEU:HD13 | 5        | 0.13          |
| (1,4196) | 1:162:B:THR:H    | 1:102:B:ASN:HB2  | 5        | 0.13          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG21 | 2        | 0.13          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG22 | 2        | 0.13          |
| (1,4168) | 1:158:B:SER:H    | 1:162:B:THR:HG23 | 2        | 0.13          |
| (1,4160) | 1:158:B:SER:H    | 1:157:B:LEU:HG   | 5        | 0.13          |
| (1,4158) | 1:158:B:SER:H    | 1:109:B:LEU:HD11 | 9        | 0.13          |
| (1,4158) | 1:158:B:SER:H    | 1:109:B:LEU:HD12 | 9        | 0.13          |
| (1,4158) | 1:158:B:SER:H    | 1:109:B:LEU:HD13 | 9        | 0.13          |
| (1,4096) | 1:153:B:VAL:H    | 1:113:B:THR:HG21 | 2        | 0.13          |
| (1,4096) | 1:153:B:VAL:H    | 1:113:B:THR:HG22 | 2        | 0.13          |
| (1,4096) | 1:153:B:VAL:H    | 1:113:B:THR:HG23 | 2        | 0.13          |
| (1,4089) | 1:152:B:GLN:HE22 | 1:152:B:GLN:HB2  | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 2        | 0.13          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 2        | 0.13          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 2        | 0.13          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG21 | 8        | 0.13          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG22 | 8        | 0.13          |
| (1,4078) | 1:152:B:GLN:HE21 | 1:151:B:THR:HG23 | 8        | 0.13          |
| (1,4043) | 1:149:B:ASP:H    | 1:152:B:GLN:HB2  | 4        | 0.13          |
| (1,4043) | 1:149:B:ASP:H    | 1:152:B:GLN:HB2  | 10       | 0.13          |
| (1,4034) | 1:148:B:VAL:H    | 1:149:B:ASP:H    | 1        | 0.13          |
| (1,3935) | 1:134:B:ILE:H    | 1:127:B:ARG:HB2  | 9        | 0.13          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE1  | 4        | 0.13          |
| (1,3932) | 1:132:B:GLY:H    | 1:133:B:TYR:HE2  | 4        | 0.13          |
| (1,3928) | 1:132:B:GLY:H    | 1:131:B:HIS:HB3  | 7        | 0.13          |
| (1,3928) | 1:132:B:GLY:H    | 1:131:B:HIS:HB3  | 8        | 0.13          |
| (1,3881) | 1:128:B:GLN:H    | 1:127:B:ARG:HD2  | 8        | 0.13          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD1  | 5        | 0.13          |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD2  | 5        | 0.13          |
| (1,3848) | 1:123:B:LYS:H    | 1:109:B:LEU:HG   | 3        | 0.13          |
| (1,3834) | 1:121:B:THR:H    | 1:120:B:ILE:HG13 | 9        | 0.13          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD11 | 8        | 0.13          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD12 | 8        | 0.13          |
| (1,3821) | 1:120:B:ILE:H    | 1:120:B:ILE:HD13 | 8        | 0.13          |
| (1,3806) | 1:119:B:GLU:H    | 1:114:B:LYS:HB3  | 2        | 0.13          |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 4        | 0.13          |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 2        | 0.13          |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 8        | 0.13          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG21 | 5        | 0.13          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG22 | 5        | 0.13          |
| (1,3787) | 1:117:B:VAL:H    | 1:118:B:VAL:HG23 | 5        | 0.13          |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG21 | 2        | 0.13          |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG22 | 2        | 0.13          |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG23 | 2        | 0.13          |
| (1,3770) | 1:114:B:LYS:H    | 1:119:B:GLU:H    | 6        | 0.13          |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD21 | 2        | 0.13          |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD22 | 2        | 0.13          |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD23 | 2        | 0.13          |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD11 | 9        | 0.13          |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD12 | 9        | 0.13          |
| (1,3702) | 1:108:B:GLU:H    | 1:109:B:LEU:HD13 | 9        | 0.13          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 5        | 0.13          |
| (1,3614) | 1:95:B:TRP:H     | 1:166:B:GLU:HG3  | 7        | 0.13          |
| (1,3608) | 1:94:B:ARG:H     | 1:169:B:MET:HG2  | 9        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 10       | 0.13          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 7        | 0.13          |
| (1,3479) | 1:159:B:PRO:HA   | 1:159:B:PRO:HB3  | 7        | 0.13          |
| (1,3478) | 1:158:B:SER:HB3  | 1:159:B:PRO:HD3  | 2        | 0.13          |
| (1,3474) | 1:158:B:SER:HB3  | 1:160:B:GLU:HB3  | 4        | 0.13          |
| (1,3474) | 1:158:B:SER:HB3  | 1:160:B:GLU:HB3  | 10       | 0.13          |
| (1,3454) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB3  | 6        | 0.13          |
| (1,3454) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB3  | 6        | 0.13          |
| (1,3454) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB3  | 6        | 0.13          |
| (1,3438) | 1:157:B:LEU:HB3  | 1:157:B:LEU:HG   | 1        | 0.13          |
| (1,3385) | 1:155:B:SER:HA   | 1:156:B:SER:HB3  | 3        | 0.13          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG21 | 9        | 0.13          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG22 | 9        | 0.13          |
| (1,3381) | 1:154:B:SER:HB2  | 1:165:B:VAL:HG23 | 9        | 0.13          |
| (1,3360) | 1:153:B:VAL:HB   | 1:154:B:SER:HA   | 5        | 0.13          |
| (1,3358) | 1:153:B:VAL:HA   | 1:168:B:PRO:HD2  | 7        | 0.13          |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 7        | 0.13          |
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 7        | 0.13          |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 7        | 0.13          |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 10       | 0.13          |
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 10       | 0.13          |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 10       | 0.13          |
| (1,3258) | 1:147:B:GLY:HA3  | 1:148:B:VAL:HB   | 9        | 0.13          |
| (1,3249) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA3  | 7        | 0.13          |
| (1,3239) | 1:145:B:PRO:HG3  | 1:146:B:PRO:HD2  | 5        | 0.13          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 10       | 0.13          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 10       | 0.13          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 10       | 0.13          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 3        | 0.13          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 3        | 0.13          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 3        | 0.13          |
| (1,3163) | 1:142:B:TYR:HD1  | 1:165:B:VAL:HG11 | 2        | 0.13          |
| (1,3163) | 1:142:B:TYR:HD1  | 1:165:B:VAL:HG12 | 2        | 0.13          |
| (1,3163) | 1:142:B:TYR:HD1  | 1:165:B:VAL:HG13 | 2        | 0.13          |
| (1,3163) | 1:142:B:TYR:HD2  | 1:165:B:VAL:HG11 | 2        | 0.13          |
| (1,3163) | 1:142:B:TYR:HD2  | 1:165:B:VAL:HG12 | 2        | 0.13          |
| (1,3163) | 1:142:B:TYR:HD2  | 1:165:B:VAL:HG13 | 2        | 0.13          |
| (1,3153) | 1:142:B:TYR:HB2  | 1:143:B:THR:HB   | 5        | 0.13          |
| (1,3143) | 1:141:B:LYS:HG3  | 1:142:B:TYR:HB3  | 5        | 0.13          |
| (1,3133) | 1:141:B:LYS:HG2  | 1:141:B:LYS:HE2  | 2        | 0.13          |
| (1,3093) | 1:136:B:ARG:HA   | 1:136:B:ARG:HD2  | 10       | 0.13          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD1  | 3        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD2  | 3        | 0.13          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD1  | 3        | 0.13          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD2  | 3        | 0.13          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD1  | 3        | 0.13          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD2  | 3        | 0.13          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD1  | 10       | 0.13          |
| (1,3078) | 1:134:B:ILE:HG21 | 1:133:B:TYR:HD2  | 10       | 0.13          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD1  | 10       | 0.13          |
| (1,3078) | 1:134:B:ILE:HG22 | 1:133:B:TYR:HD2  | 10       | 0.13          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD1  | 10       | 0.13          |
| (1,3078) | 1:134:B:ILE:HG23 | 1:133:B:TYR:HD2  | 10       | 0.13          |
| (1,3048) | 1:129:B:ASP:HA   | 1:133:B:TYR:HA   | 4        | 0.13          |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD1  | 9        | 0.13          |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD2  | 9        | 0.13          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE1  | 5        | 0.13          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE2  | 5        | 0.13          |
| (1,3015) | 1:127:B:ARG:HA   | 1:127:B:ARG:HB3  | 1        | 0.13          |
| (1,3015) | 1:127:B:ARG:HA   | 1:127:B:ARG:HB3  | 9        | 0.13          |
| (1,2985) | 1:125:B:GLU:HA   | 1:135:B:SER:HB3  | 2        | 0.13          |
| (1,2963) | 1:123:B:LYS:HA   | 1:123:B:LYS:HE2  | 7        | 0.13          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 10       | 0.13          |
| (1,2933) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HB2  | 4        | 0.13          |
| (1,2933) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HB2  | 4        | 0.13          |
| (1,2933) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HB2  | 4        | 0.13          |
| (1,2928) | 1:120:B:ILE:HG21 | 1:122:B:GLY:HA3  | 7        | 0.13          |
| (1,2928) | 1:120:B:ILE:HG22 | 1:122:B:GLY:HA3  | 7        | 0.13          |
| (1,2928) | 1:120:B:ILE:HG23 | 1:122:B:GLY:HA3  | 7        | 0.13          |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 5        | 0.13          |
| (1,2885) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG12 | 5        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 7        | 0.13          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 7        | 0.13          |
| (1,2866) | 1:118:B:VAL:HG11 | 1:142:B:TYR:HD1  | 9        | 0.13          |
| (1,2866) | 1:118:B:VAL:HG11 | 1:142:B:TYR:HD2  | 9        | 0.13          |
| (1,2866) | 1:118:B:VAL:HG12 | 1:142:B:TYR:HD1  | 9        | 0.13          |
| (1,2866) | 1:118:B:VAL:HG12 | 1:142:B:TYR:HD2  | 9        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2866) | 1:118:B:VAL:HG13 | 1:142:B:TYR:HD1  | 9        | 0.13          |
| (1,2866) | 1:118:B:VAL:HG13 | 1:142:B:TYR:HD2  | 9        | 0.13          |
| (1,2858) | 1:118:B:VAL:HB   | 1:153:B:VAL:HG21 | 5        | 0.13          |
| (1,2858) | 1:118:B:VAL:HB   | 1:153:B:VAL:HG22 | 5        | 0.13          |
| (1,2858) | 1:118:B:VAL:HB   | 1:153:B:VAL:HG23 | 5        | 0.13          |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD21 | 9        | 0.13          |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD22 | 9        | 0.13          |
| (1,2847) | 1:118:B:VAL:HA   | 1:144:B:LEU:HD23 | 9        | 0.13          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG21 | 6        | 0.13          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG22 | 6        | 0.13          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG23 | 6        | 0.13          |
| (1,2798) | 1:115:B:ASP:HB3  | 1:150:B:PRO:HG2  | 2        | 0.13          |
| (1,2754) | 1:112:B:LYS:HE2  | 1:114:B:LYS:HB2  | 10       | 0.13          |
| (1,2753) | 1:112:B:LYS:HD2  | 1:120:B:ILE:HA   | 9        | 0.13          |
| (1,2740) | 1:112:B:LYS:HB3  | 1:112:B:LYS:HE2  | 6        | 0.13          |
| (1,2738) | 1:112:B:LYS:HB2  | 1:120:B:ILE:HA   | 4        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG21 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG22 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG23 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG21 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG22 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG23 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG21 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG22 | 1        | 0.13          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG23 | 1        | 0.13          |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 1        | 0.13          |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 10       | 0.13          |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD21 | 8        | 0.13          |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD22 | 8        | 0.13          |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD23 | 8        | 0.13          |
| (1,2640) | 1:109:B:LEU:HB2  | 1:122:B:GLY:HA2  | 4        | 0.13          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD11 | 7        | 0.13          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD12 | 7        | 0.13          |
| (1,2639) | 1:109:B:LEU:HB2  | 1:109:B:LEU:HD13 | 7        | 0.13          |
| (1,2613) | 1:107:B:ASP:HA   | 1:108:B:GLU:HG3  | 1        | 0.13          |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD11 | 7        | 0.13          |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD12 | 7        | 0.13          |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD13 | 7        | 0.13          |
| (1,2564) | 1:105:B:ALA:HA   | 1:106:B:PRO:HB3  | 7        | 0.13          |
| (1,2559) | 1:102:B:ASN:HB2  | 1:161:B:GLY:HA3  | 4        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG11  | 1:99:B:LEU:HD21  | 8        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG11  | 1:99:B:LEU:HD22  | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2446) | 1:97:B:VAL:HG11 | 1:99:B:LEU:HD23  | 8        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG12 | 1:99:B:LEU:HD21  | 8        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG12 | 1:99:B:LEU:HD22  | 8        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG12 | 1:99:B:LEU:HD23  | 8        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG13 | 1:99:B:LEU:HD21  | 8        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG13 | 1:99:B:LEU:HD22  | 8        | 0.13          |
| (1,2446) | 1:97:B:VAL:HG13 | 1:99:B:LEU:HD23  | 8        | 0.13          |
| (1,2422) | 1:97:B:VAL:HG11 | 1:142:B:TYR:HD1  | 8        | 0.13          |
| (1,2422) | 1:97:B:VAL:HG11 | 1:142:B:TYR:HD2  | 8        | 0.13          |
| (1,2422) | 1:97:B:VAL:HG12 | 1:142:B:TYR:HD1  | 8        | 0.13          |
| (1,2422) | 1:97:B:VAL:HG12 | 1:142:B:TYR:HD2  | 8        | 0.13          |
| (1,2422) | 1:97:B:VAL:HG13 | 1:142:B:TYR:HD1  | 8        | 0.13          |
| (1,2422) | 1:97:B:VAL:HG13 | 1:142:B:TYR:HD2  | 8        | 0.13          |
| (1,2413) | 1:97:B:VAL:HB   | 1:165:B:VAL:HG21 | 10       | 0.13          |
| (1,2413) | 1:97:B:VAL:HB   | 1:165:B:VAL:HG22 | 10       | 0.13          |
| (1,2413) | 1:97:B:VAL:HB   | 1:165:B:VAL:HG23 | 10       | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG11 | 2        | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG12 | 2        | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG13 | 2        | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG11 | 3        | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG12 | 3        | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG13 | 3        | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG11 | 10       | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG12 | 10       | 0.13          |
| (1,2410) | 1:97:B:VAL:HB   | 1:148:B:VAL:HG13 | 10       | 0.13          |
| (1,2400) | 1:97:B:VAL:HA   | 1:97:B:VAL:HG11  | 10       | 0.13          |
| (1,2400) | 1:97:B:VAL:HA   | 1:97:B:VAL:HG12  | 10       | 0.13          |
| (1,2400) | 1:97:B:VAL:HA   | 1:97:B:VAL:HG13  | 10       | 0.13          |
| (1,2382) | 1:96:B:ARG:HB3  | 1:166:B:GLU:HA   | 6        | 0.13          |
| (1,2357) | 1:95:B:TRP:HE3  | 1:166:B:GLU:HA   | 8        | 0.13          |
| (1,2349) | 1:95:B:TRP:HB3  | 1:148:B:VAL:HG21 | 2        | 0.13          |
| (1,2349) | 1:95:B:TRP:HB3  | 1:148:B:VAL:HG22 | 2        | 0.13          |
| (1,2349) | 1:95:B:TRP:HB3  | 1:148:B:VAL:HG23 | 2        | 0.13          |
| (1,2329) | 1:94:B:ARG:HD2  | 1:168:B:PRO:HA   | 4        | 0.13          |
| (1,2326) | 1:94:B:ARG:HG2  | 1:168:B:PRO:HB2  | 2        | 0.13          |
| (1,2326) | 1:94:B:ARG:HG2  | 1:168:B:PRO:HB2  | 3        | 0.13          |
| (1,2326) | 1:94:B:ARG:HG2  | 1:168:B:PRO:HB2  | 6        | 0.13          |
| (1,2326) | 1:94:B:ARG:HG2  | 1:168:B:PRO:HB2  | 10       | 0.13          |
| (1,2315) | 1:94:B:ARG:HB2  | 1:94:B:ARG:HG2   | 9        | 0.13          |
| (1,2304) | 1:94:B:ARG:HA   | 1:94:B:ARG:HB3   | 8        | 0.13          |
| (1,2292) | 1:91:B:THR:HB   | 1:92:B:ALA:HB1   | 8        | 0.13          |
| (1,2292) | 1:91:B:THR:HB   | 1:92:B:ALA:HB2   | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2292) | 1:91:B:THR:HB    | 1:92:B:ALA:HB3   | 8        | 0.13          |
| (1,2225) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 5        | 0.13          |
| (1,2225) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 5        | 0.13          |
| (1,2225) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 5        | 0.13          |
| (1,2093) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 5        | 0.13          |
| (1,2093) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 5        | 0.13          |
| (1,2093) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 5        | 0.13          |
| (1,2016) | 1:174:A:THR:H    | 1:171:A:LYS:HG3  | 5        | 0.13          |
| (1,2000) | 1:169:A:MET:H    | 1:169:A:MET:HG3  | 5        | 0.13          |
| (1,1981) | 1:167:A:ALA:H    | 1:166:A:GLU:HB2  | 3        | 0.13          |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD11 | 5        | 0.13          |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD12 | 5        | 0.13          |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD13 | 5        | 0.13          |
| (1,1935) | 1:163:A:LEU:H    | 1:164:A:THR:H    | 2        | 0.13          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 3        | 0.13          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 9        | 0.13          |
| (1,1902) | 1:161:A:GLY:H    | 1:102:A:ASN:HB3  | 8        | 0.13          |
| (1,1901) | 1:161:A:GLY:H    | 1:102:A:ASN:HB2  | 1        | 0.13          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG21 | 7        | 0.13          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG22 | 7        | 0.13          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG23 | 7        | 0.13          |
| (1,1849) | 1:155:A:SER:H    | 1:156:A:SER:HA   | 7        | 0.13          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 2        | 0.13          |
| (1,1796) | 1:152:A:GLN:HE21 | 1:149:A:ASP:HB2  | 7        | 0.13          |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 3        | 0.13          |
| (1,1751) | 1:148:A:VAL:H    | 1:149:A:ASP:HA   | 6        | 0.13          |
| (1,1744) | 1:148:A:VAL:H    | 1:146:A:PRO:HG2  | 9        | 0.13          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 10       | 0.13          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 10       | 0.13          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 10       | 0.13          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD11  | 9        | 0.13          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD12  | 9        | 0.13          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD13  | 9        | 0.13          |
| (1,1669) | 1:136:A:ARG:H    | 1:134:A:ILE:HG21 | 2        | 0.13          |
| (1,1669) | 1:136:A:ARG:H    | 1:134:A:ILE:HG22 | 2        | 0.13          |
| (1,1669) | 1:136:A:ARG:H    | 1:134:A:ILE:HG23 | 2        | 0.13          |
| (1,1654) | 1:134:A:ILE:H    | 1:127:A:ARG:HB2  | 8        | 0.13          |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG3  | 4        | 0.13          |
| (1,1627) | 1:129:A:ASP:H    | 1:132:A:GLY:H    | 3        | 0.13          |
| (1,1617) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HG3  | 6        | 0.13          |
| (1,1588) | 1:126:A:GLU:H    | 1:125:A:GLU:HG3  | 1        | 0.13          |
| (1,1588) | 1:126:A:GLU:H    | 1:125:A:GLU:HG3  | 9        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD11 | 8        | 0.13          |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD12 | 8        | 0.13          |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD13 | 8        | 0.13          |
| (1,1525) | 1:119:A:GLU:H    | 1:114:A:LYS:HB3  | 7        | 0.13          |
| (1,1467) | 1:113:A:THR:H    | 1:112:A:LYS:HB2  | 3        | 0.13          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD11 | 2        | 0.13          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD12 | 2        | 0.13          |
| (1,1449) | 1:111:A:VAL:H    | 1:120:A:ILE:HD13 | 2        | 0.13          |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD21 | 5        | 0.13          |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD22 | 5        | 0.13          |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD23 | 5        | 0.13          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD21 | 3        | 0.13          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD22 | 3        | 0.13          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD23 | 3        | 0.13          |
| (1,1373) | 1:102:A:ASN:HD21 | 1:161:A:GLY:HA2  | 4        | 0.13          |
| (1,1362) | 1:101:A:VAL:H    | 1:120:A:ILE:HG21 | 1        | 0.13          |
| (1,1362) | 1:101:A:VAL:H    | 1:120:A:ILE:HG22 | 1        | 0.13          |
| (1,1362) | 1:101:A:VAL:H    | 1:120:A:ILE:HG23 | 1        | 0.13          |
| (1,1345) | 1:97:A:VAL:H     | 1:165:A:VAL:H    | 3        | 0.13          |
| (1,1328) | 1:94:A:ARG:H     | 1:169:A:MET:HG3  | 8        | 0.13          |
| (1,1311) | 1:170:A:PRO:HB2  | 1:170:A:PRO:HG2  | 9        | 0.13          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 9        | 0.13          |
| (1,1285) | 1:168:A:PRO:HD2  | 1:169:A:MET:HA   | 5        | 0.13          |
| (1,1217) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HA   | 5        | 0.13          |
| (1,1174) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HG   | 8        | 0.13          |
| (1,1174) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HG   | 8        | 0.13          |
| (1,1174) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HG   | 8        | 0.13          |
| (1,1172) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB2  | 7        | 0.13          |
| (1,1172) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB2  | 7        | 0.13          |
| (1,1172) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB2  | 7        | 0.13          |
| (1,1168) | 1:157:A:LEU:HD11 | 1:161:A:GLY:HA3  | 6        | 0.13          |
| (1,1168) | 1:157:A:LEU:HD12 | 1:161:A:GLY:HA3  | 6        | 0.13          |
| (1,1168) | 1:157:A:LEU:HD13 | 1:161:A:GLY:HA3  | 6        | 0.13          |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 5        | 0.13          |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 7        | 0.13          |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 9        | 0.13          |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 3        | 0.13          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD21 | 5        | 0.13          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD22 | 5        | 0.13          |
| (1,1141) | 1:156:A:SER:HB3  | 1:163:A:LEU:HD23 | 5        | 0.13          |
| (1,1128) | 1:155:A:SER:HB2  | 1:157:A:LEU:HB3  | 6        | 0.13          |
| (1,1110) | 1:155:A:SER:HA   | 1:165:A:VAL:HA   | 2        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1110) | 1:155:A:SER:HA   | 1:165:A:VAL:HA   | 8        | 0.13          |
| (1,1079) | 1:153:A:VAL:HB   | 1:154:A:SER:HA   | 6        | 0.13          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 7        | 0.13          |
| (1,1028) | 1:149:A:ASP:HA   | 1:150:A:PRO:HD3  | 8        | 0.13          |
| (1,1020) | 1:148:A:VAL:HG21 | 1:169:A:MET:HB2  | 4        | 0.13          |
| (1,1020) | 1:148:A:VAL:HG22 | 1:169:A:MET:HB2  | 4        | 0.13          |
| (1,1020) | 1:148:A:VAL:HG23 | 1:169:A:MET:HB2  | 4        | 0.13          |
| (1,857)  | 1:141:A:LYS:HG2  | 1:143:A:THR:HA   | 10       | 0.13          |
| (1,852)  | 1:141:A:LYS:HG2  | 1:141:A:LYS:HE2  | 2        | 0.13          |
| (1,852)  | 1:141:A:LYS:HG2  | 1:141:A:LYS:HE2  | 9        | 0.13          |
| (1,812)  | 1:136:A:ARG:HA   | 1:136:A:ARG:HD2  | 3        | 0.13          |
| (1,812)  | 1:136:A:ARG:HA   | 1:136:A:ARG:HD2  | 4        | 0.13          |
| (1,782)  | 1:131:A:HIS:HB2  | 1:132:A:GLY:HA2  | 2        | 0.13          |
| (1,729)  | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 1        | 0.13          |
| (1,704)  | 1:125:A:GLU:HA   | 1:135:A:SER:HB3  | 4        | 0.13          |
| (1,684)  | 1:123:A:LYS:HA   | 1:135:A:SER:HB3  | 8        | 0.13          |
| (1,682)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HE3  | 10       | 0.13          |
| (1,680)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 1        | 0.13          |
| (1,658)  | 1:120:A:ILE:HD11 | 1:163:A:LEU:HA   | 1        | 0.13          |
| (1,658)  | 1:120:A:ILE:HD12 | 1:163:A:LEU:HA   | 1        | 0.13          |
| (1,658)  | 1:120:A:ILE:HD13 | 1:163:A:LEU:HA   | 1        | 0.13          |
| (1,654)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD2  | 1        | 0.13          |
| (1,654)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD2  | 1        | 0.13          |
| (1,654)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD2  | 1        | 0.13          |
| (1,654)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD2  | 4        | 0.13          |
| (1,654)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD2  | 4        | 0.13          |
| (1,654)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD2  | 4        | 0.13          |
| (1,652)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HB2  | 1        | 0.13          |
| (1,652)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HB2  | 1        | 0.13          |
| (1,652)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HB2  | 1        | 0.13          |
| (1,652)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HB2  | 5        | 0.13          |
| (1,652)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HB2  | 5        | 0.13          |
| (1,652)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HB2  | 5        | 0.13          |
| (1,647)  | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 4        | 0.13          |
| (1,647)  | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 4        | 0.13          |
| (1,647)  | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 4        | 0.13          |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD11 | 2        | 0.13          |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD12 | 2        | 0.13          |
| (1,640)  | 1:120:A:ILE:HG12 | 1:163:A:LEU:HD13 | 2        | 0.13          |
| (1,639)  | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 4        | 0.13          |
| (1,608)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HA   | 4        | 0.13          |
| (1,605)  | 1:119:A:GLU:HA   | 1:120:A:ILE:HG13 | 5        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,590) | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG11 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG12 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG11 | 1:148:A:VAL:HG13 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG11 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG12 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG12 | 1:148:A:VAL:HG13 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG11 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG12 | 4        | 0.13          |
| (1,590) | 1:118:A:VAL:HG13 | 1:148:A:VAL:HG13 | 4        | 0.13          |
| (1,571) | 1:118:A:VAL:HB   | 1:142:A:TYR:HD1  | 1        | 0.13          |
| (1,571) | 1:118:A:VAL:HB   | 1:142:A:TYR:HD2  | 1        | 0.13          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD21 | 5        | 0.13          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD22 | 5        | 0.13          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD23 | 5        | 0.13          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG21 | 10       | 0.13          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG22 | 10       | 0.13          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG23 | 10       | 0.13          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG21 | 4        | 0.13          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG22 | 4        | 0.13          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG23 | 4        | 0.13          |
| (1,449) | 1:112:A:LYS:HA   | 1:112:A:LYS:HE3  | 6        | 0.13          |
| (1,419) | 1:111:A:VAL:HA   | 1:120:A:ILE:HG13 | 7        | 0.13          |
| (1,418) | 1:111:A:VAL:HA   | 1:120:A:ILE:HG12 | 1        | 0.13          |
| (1,415) | 1:111:A:VAL:HA   | 1:112:A:LYS:HE3  | 1        | 0.13          |
| (1,405) | 1:110:A:THR:HG21 | 1:112:A:LYS:HD3  | 5        | 0.13          |
| (1,405) | 1:110:A:THR:HG22 | 1:112:A:LYS:HD3  | 5        | 0.13          |
| (1,405) | 1:110:A:THR:HG23 | 1:112:A:LYS:HD3  | 5        | 0.13          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD21 | 9        | 0.13          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD22 | 9        | 0.13          |
| (1,361) | 1:109:A:LEU:HB3  | 1:109:A:LEU:HD23 | 9        | 0.13          |
| (1,348) | 1:108:A:GLU:HG3  | 1:123:A:LYS:HE2  | 10       | 0.13          |
| (1,331) | 1:107:A:ASP:HA   | 1:108:A:GLU:HG2  | 7        | 0.13          |
| (1,279) | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA2  | 3        | 0.13          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 1        | 0.13          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 1        | 0.13          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 1        | 0.13          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD11 | 3        | 0.13          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD12 | 3        | 0.13          |
| (1,269) | 1:101:A:VAL:HB   | 1:157:A:LEU:HD13 | 3        | 0.13          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG21 | 3        | 0.13          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG22 | 3        | 0.13          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG23 | 3        | 0.13          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,259) | 1:100:A:ASP:HA  | 1:100:A:ASP:HB3  | 2        | 0.13          |
| (1,236) | 1:99:A:LEU:HD11 | 1:164:A:THR:HA   | 4        | 0.13          |
| (1,236) | 1:99:A:LEU:HD12 | 1:164:A:THR:HA   | 4        | 0.13          |
| (1,236) | 1:99:A:LEU:HD13 | 1:164:A:THR:HA   | 4        | 0.13          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG11 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG12 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG13 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG11 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG12 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG13 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG11 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG12 | 3        | 0.13          |
| (1,229) | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG13 | 3        | 0.13          |
| (1,226) | 1:99:A:LEU:HD11 | 1:101:A:VAL:HG21 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD11 | 1:101:A:VAL:HG22 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD11 | 1:101:A:VAL:HG23 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG21 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG22 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG23 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG21 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG22 | 7        | 0.13          |
| (1,226) | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG23 | 7        | 0.13          |
| (1,187) | 1:98:A:SER:HB2  | 1:164:A:THR:HB   | 3        | 0.13          |
| (1,176) | 1:98:A:SER:HA   | 1:162:A:THR:HG21 | 3        | 0.13          |
| (1,176) | 1:98:A:SER:HA   | 1:162:A:THR:HG22 | 3        | 0.13          |
| (1,176) | 1:98:A:SER:HA   | 1:162:A:THR:HG23 | 3        | 0.13          |
| (1,141) | 1:97:A:VAL:HG11 | 1:142:A:TYR:HD1  | 6        | 0.13          |
| (1,141) | 1:97:A:VAL:HG11 | 1:142:A:TYR:HD2  | 6        | 0.13          |
| (1,141) | 1:97:A:VAL:HG12 | 1:142:A:TYR:HD1  | 6        | 0.13          |
| (1,141) | 1:97:A:VAL:HG12 | 1:142:A:TYR:HD2  | 6        | 0.13          |
| (1,141) | 1:97:A:VAL:HG13 | 1:142:A:TYR:HD1  | 6        | 0.13          |
| (1,141) | 1:97:A:VAL:HG13 | 1:142:A:TYR:HD2  | 6        | 0.13          |
| (1,108) | 1:96:A:ARG:HG2  | 1:97:A:VAL:HG21  | 4        | 0.13          |
| (1,108) | 1:96:A:ARG:HG2  | 1:97:A:VAL:HG22  | 4        | 0.13          |
| (1,108) | 1:96:A:ARG:HG2  | 1:97:A:VAL:HG23  | 4        | 0.13          |
| (1,88)  | 1:96:A:ARG:HA   | 1:165:A:VAL:HG21 | 5        | 0.13          |
| (1,88)  | 1:96:A:ARG:HA   | 1:165:A:VAL:HG22 | 5        | 0.13          |
| (1,88)  | 1:96:A:ARG:HA   | 1:165:A:VAL:HG23 | 5        | 0.13          |
| (1,80)  | 1:96:A:ARG:HA   | 1:96:A:ARG:HD3   | 3        | 0.13          |
| (1,68)  | 1:95:A:TRP:HB3  | 1:148:A:VAL:HG21 | 6        | 0.13          |
| (1,68)  | 1:95:A:TRP:HB3  | 1:148:A:VAL:HG22 | 6        | 0.13          |
| (1,68)  | 1:95:A:TRP:HB3  | 1:148:A:VAL:HG23 | 6        | 0.13          |

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| Key      | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|----------|---------------|------------------|----------|---------------|
| (1,33)   | 1:94:A:ARG:HA | 1:169:A:MET:HB2  | 9        | 0.13          |
| (1,32)   | 1:94:A:ARG:HA | 1:168:A:PRO:HD3  | 2        | 0.13          |
| (1,23)   | 1:94:A:ARG:HA | 1:94:A:ARG:HB3   | 3        | 0.13          |
| (1,23)   | 1:94:A:ARG:HA | 1:94:A:ARG:HB3   | 4        | 0.13          |
| (1,23)   | 1:94:A:ARG:HA | 1:94:A:ARG:HB3   | 10       | 0.13          |
| (1,4297) | 1:174:B:THR:H | 1:171:B:LYS:HG3  | 9        | 0.12          |
| (1,4263) | 1:167:B:ALA:H | 1:166:B:GLU:HB3  | 3        | 0.12          |
| (1,4263) | 1:167:B:ALA:H | 1:166:B:GLU:HB3  | 9        | 0.12          |
| (1,4262) | 1:167:B:ALA:H | 1:166:B:GLU:HB2  | 7        | 0.12          |
| (1,4239) | 1:165:B:VAL:H | 1:166:B:GLU:HB3  | 7        | 0.12          |
| (1,4234) | 1:165:B:VAL:H | 1:153:B:VAL:HG11 | 9        | 0.12          |
| (1,4234) | 1:165:B:VAL:H | 1:153:B:VAL:HG12 | 9        | 0.12          |
| (1,4234) | 1:165:B:VAL:H | 1:153:B:VAL:HG13 | 9        | 0.12          |
| (1,4219) | 1:164:B:THR:H | 1:157:B:LEU:HD11 | 4        | 0.12          |
| (1,4219) | 1:164:B:THR:H | 1:157:B:LEU:HD12 | 4        | 0.12          |
| (1,4219) | 1:164:B:THR:H | 1:157:B:LEU:HD13 | 4        | 0.12          |
| (1,4219) | 1:164:B:THR:H | 1:157:B:LEU:HD11 | 7        | 0.12          |
| (1,4219) | 1:164:B:THR:H | 1:157:B:LEU:HD12 | 7        | 0.12          |
| (1,4219) | 1:164:B:THR:H | 1:157:B:LEU:HD13 | 7        | 0.12          |
| (1,4216) | 1:163:B:LEU:H | 1:164:B:THR:H    | 9        | 0.12          |
| (1,4190) | 1:161:B:GLY:H | 1:160:B:GLU:HB3  | 5        | 0.12          |
| (1,4183) | 1:161:B:GLY:H | 1:102:B:ASN:HB3  | 6        | 0.12          |
| (1,4175) | 1:160:B:GLU:H | 1:159:B:PRO:HG2  | 9        | 0.12          |
| (1,4158) | 1:158:B:SER:H | 1:109:B:LEU:HD11 | 1        | 0.12          |
| (1,4158) | 1:158:B:SER:H | 1:109:B:LEU:HD12 | 1        | 0.12          |
| (1,4158) | 1:158:B:SER:H | 1:109:B:LEU:HD13 | 1        | 0.12          |
| (1,4047) | 1:149:B:ASP:H | 1:169:B:MET:HG3  | 6        | 0.12          |
| (1,4032) | 1:148:B:VAL:H | 1:149:B:ASP:HA   | 5        | 0.12          |
| (1,3955) | 1:137:B:CYS:H | 1:136:B:ARG:HB3  | 5        | 0.12          |
| (1,3948) | 1:135:B:SER:H | 1:135:B:SER:HB2  | 4        | 0.12          |
| (1,3928) | 1:132:B:GLY:H | 1:131:B:HIS:HB3  | 9        | 0.12          |
| (1,3923) | 1:132:B:GLY:H | 1:129:B:ASP:HB2  | 6        | 0.12          |
| (1,3903) | 1:129:B:ASP:H | 1:129:B:ASP:HB3  | 5        | 0.12          |
| (1,3860) | 1:124:B:HIS:H | 1:138:B:PHE:HD1  | 2        | 0.12          |
| (1,3860) | 1:124:B:HIS:H | 1:138:B:PHE:HD2  | 2        | 0.12          |
| (1,3850) | 1:123:B:LYS:H | 1:109:B:LEU:HD21 | 1        | 0.12          |
| (1,3850) | 1:123:B:LYS:H | 1:109:B:LEU:HD22 | 1        | 0.12          |
| (1,3850) | 1:123:B:LYS:H | 1:109:B:LEU:HD23 | 1        | 0.12          |
| (1,3837) | 1:121:B:THR:H | 1:121:B:THR:HG21 | 7        | 0.12          |
| (1,3837) | 1:121:B:THR:H | 1:121:B:THR:HG22 | 7        | 0.12          |
| (1,3837) | 1:121:B:THR:H | 1:121:B:THR:HG23 | 7        | 0.12          |
| (1,3837) | 1:121:B:THR:H | 1:121:B:THR:HG21 | 8        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG22 | 8        | 0.12          |
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG23 | 8        | 0.12          |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 2        | 0.12          |
| (1,3790) | 1:117:B:VAL:H    | 1:144:B:LEU:H    | 6        | 0.12          |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG21 | 6        | 0.12          |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG22 | 6        | 0.12          |
| (1,3786) | 1:117:B:VAL:H    | 1:117:B:VAL:HG23 | 6        | 0.12          |
| (1,3723) | 1:110:B:THR:H    | 1:122:B:GLY:H    | 9        | 0.12          |
| (1,3720) | 1:110:B:THR:H    | 1:120:B:ILE:HD11 | 9        | 0.12          |
| (1,3720) | 1:110:B:THR:H    | 1:120:B:ILE:HD12 | 9        | 0.12          |
| (1,3720) | 1:110:B:THR:H    | 1:120:B:ILE:HD13 | 9        | 0.12          |
| (1,3692) | 1:108:B:GLU:H    | 1:105:B:ALA:HA   | 2        | 0.12          |
| (1,3670) | 1:105:B:ALA:H    | 1:106:B:PRO:HD3  | 7        | 0.12          |
| (1,3670) | 1:105:B:ALA:H    | 1:106:B:PRO:HD3  | 10       | 0.12          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD21 | 5        | 0.12          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD22 | 5        | 0.12          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD23 | 5        | 0.12          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD21 | 6        | 0.12          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD22 | 6        | 0.12          |
| (1,3665) | 1:103:B:HIS:H    | 1:109:B:LEU:HD23 | 6        | 0.12          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD11 | 9        | 0.12          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD12 | 9        | 0.12          |
| (1,3661) | 1:102:B:ASN:HD22 | 1:157:B:LEU:HD13 | 9        | 0.12          |
| (1,3655) | 1:102:B:ASN:HD21 | 1:161:B:GLY:HA3  | 10       | 0.12          |
| (1,3651) | 1:102:B:ASN:HD21 | 1:109:B:LEU:HD21 | 10       | 0.12          |
| (1,3651) | 1:102:B:ASN:HD21 | 1:109:B:LEU:HD22 | 10       | 0.12          |
| (1,3651) | 1:102:B:ASN:HD21 | 1:109:B:LEU:HD23 | 10       | 0.12          |
| (1,3592) | 1:170:B:PRO:HB2  | 1:170:B:PRO:HG2  | 3        | 0.12          |
| (1,3592) | 1:170:B:PRO:HB2  | 1:170:B:PRO:HG2  | 9        | 0.12          |
| (1,3498) | 1:161:B:GLY:HA3  | 1:163:B:LEU:HA   | 5        | 0.12          |
| (1,3487) | 1:159:B:PRO:HD2  | 1:160:B:GLU:HB3  | 7        | 0.12          |
| (1,3455) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HG   | 4        | 0.12          |
| (1,3455) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HG   | 4        | 0.12          |
| (1,3455) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HG   | 4        | 0.12          |
| (1,3438) | 1:157:B:LEU:HB3  | 1:157:B:LEU:HG   | 10       | 0.12          |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 3        | 0.12          |
| (1,3423) | 1:156:B:SER:HB3  | 1:164:B:THR:HG21 | 3        | 0.12          |
| (1,3423) | 1:156:B:SER:HB3  | 1:164:B:THR:HG22 | 3        | 0.12          |
| (1,3423) | 1:156:B:SER:HB3  | 1:164:B:THR:HG23 | 3        | 0.12          |
| (1,3378) | 1:154:B:SER:HB3  | 1:155:B:SER:HA   | 3        | 0.12          |
| (1,3360) | 1:153:B:VAL:HB   | 1:154:B:SER:HA   | 6        | 0.12          |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 3        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 3        | 0.12          |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 3        | 0.12          |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 8        | 0.12          |
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 8        | 0.12          |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 8        | 0.12          |
| (1,3249) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA3  | 10       | 0.12          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 7        | 0.12          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 7        | 0.12          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 7        | 0.12          |
| (1,3186) | 1:144:B:LEU:HA   | 1:145:B:PRO:HG3  | 3        | 0.12          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD11 | 8        | 0.12          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD12 | 8        | 0.12          |
| (1,3177) | 1:143:B:THR:HB   | 1:144:B:LEU:HD13 | 8        | 0.12          |
| (1,3087) | 1:134:B:ILE:HG22 | 1:135:B:SER:HB3  | 4        | 0.12          |
| (1,3056) | 1:130:B:GLU:HG2  | 1:131:B:HIS:HD2  | 3        | 0.12          |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD1  | 4        | 0.12          |
| (1,3037) | 1:128:B:GLN:HB3  | 1:133:B:TYR:HD2  | 4        | 0.12          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE1  | 4        | 0.12          |
| (1,3035) | 1:128:B:GLN:HB2  | 1:133:B:TYR:HE2  | 4        | 0.12          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE1  | 4        | 0.12          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE2  | 4        | 0.12          |
| (1,2997) | 1:126:B:GLU:HG2  | 1:127:B:ARG:HG2  | 6        | 0.12          |
| (1,2996) | 1:126:B:GLU:HB2  | 1:135:B:SER:HB3  | 3        | 0.12          |
| (1,2996) | 1:126:B:GLU:HB2  | 1:135:B:SER:HB3  | 9        | 0.12          |
| (1,2993) | 1:126:B:GLU:HB3  | 1:133:B:TYR:HB2  | 10       | 0.12          |
| (1,2957) | 1:122:B:GLY:HA3  | 1:137:B:CYS:HA   | 2        | 0.12          |
| (1,2952) | 1:121:B:THR:HG21 | 1:137:B:CYS:HB3  | 3        | 0.12          |
| (1,2952) | 1:121:B:THR:HG22 | 1:137:B:CYS:HB3  | 3        | 0.12          |
| (1,2952) | 1:121:B:THR:HG23 | 1:137:B:CYS:HB3  | 3        | 0.12          |
| (1,2935) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HD2  | 8        | 0.12          |
| (1,2935) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HD2  | 8        | 0.12          |
| (1,2935) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HD2  | 8        | 0.12          |
| (1,2892) | 1:119:B:GLU:HA   | 1:141:B:LYS:HE2  | 2        | 0.12          |
| (1,2892) | 1:119:B:GLU:HA   | 1:141:B:LYS:HE2  | 8        | 0.12          |
| (1,2886) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG13 | 7        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD21 | 8        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD22 | 8        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG11 | 1:144:B:LEU:HD23 | 8        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD21 | 8        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD22 | 8        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG12 | 1:144:B:LEU:HD23 | 8        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD21 | 8        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD22 | 8        | 0.12          |
| (1,2869) | 1:118:B:VAL:HG13 | 1:144:B:LEU:HD23 | 8        | 0.12          |
| (1,2866) | 1:118:B:VAL:HG11 | 1:142:B:TYR:HD1  | 2        | 0.12          |
| (1,2866) | 1:118:B:VAL:HG11 | 1:142:B:TYR:HD2  | 2        | 0.12          |
| (1,2866) | 1:118:B:VAL:HG12 | 1:142:B:TYR:HD1  | 2        | 0.12          |
| (1,2866) | 1:118:B:VAL:HG12 | 1:142:B:TYR:HD2  | 2        | 0.12          |
| (1,2866) | 1:118:B:VAL:HG13 | 1:142:B:TYR:HD1  | 2        | 0.12          |
| (1,2866) | 1:118:B:VAL:HG13 | 1:142:B:TYR:HD2  | 2        | 0.12          |
| (1,2844) | 1:118:B:VAL:HA   | 1:118:B:VAL:HG11 | 2        | 0.12          |
| (1,2844) | 1:118:B:VAL:HA   | 1:118:B:VAL:HG12 | 2        | 0.12          |
| (1,2844) | 1:118:B:VAL:HA   | 1:118:B:VAL:HG13 | 2        | 0.12          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG21 | 1        | 0.12          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG22 | 1        | 0.12          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG23 | 1        | 0.12          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG21 | 5        | 0.12          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG22 | 5        | 0.12          |
| (1,2827) | 1:117:B:VAL:HA   | 1:143:B:THR:HG23 | 5        | 0.12          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG11 | 5        | 0.12          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG12 | 5        | 0.12          |
| (1,2810) | 1:116:B:GLY:HA2  | 1:148:B:VAL:HG13 | 5        | 0.12          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG21 | 7        | 0.12          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG22 | 7        | 0.12          |
| (1,2802) | 1:116:B:GLY:HA2  | 1:118:B:VAL:HG23 | 7        | 0.12          |
| (1,2798) | 1:115:B:ASP:HB3  | 1:150:B:PRO:HG2  | 7        | 0.12          |
| (1,2798) | 1:115:B:ASP:HB3  | 1:150:B:PRO:HG2  | 10       | 0.12          |
| (1,2759) | 1:112:B:LYS:HE3  | 1:121:B:THR:HB   | 8        | 0.12          |
| (1,2730) | 1:112:B:LYS:HA   | 1:112:B:LYS:HE3  | 7        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG21 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG22 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG23 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG21 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG22 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG23 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG21 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG22 | 9        | 0.12          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG23 | 9        | 0.12          |
| (1,2699) | 1:111:B:VAL:HA   | 1:120:B:ILE:HG12 | 4        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 1        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 1        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 7        | 0.12          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 7        | 0.12          |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD21 | 10       | 0.12          |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD22 | 10       | 0.12          |
| (1,2642) | 1:109:B:LEU:HB3  | 1:109:B:LEU:HD23 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB1  | 1:109:B:LEU:HD21 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB1  | 1:109:B:LEU:HD22 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB1  | 1:109:B:LEU:HD23 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB2  | 1:109:B:LEU:HD21 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB2  | 1:109:B:LEU:HD22 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB2  | 1:109:B:LEU:HD23 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB3  | 1:109:B:LEU:HD21 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB3  | 1:109:B:LEU:HD22 | 10       | 0.12          |
| (1,2582) | 1:105:B:ALA:HB3  | 1:109:B:LEU:HD23 | 10       | 0.12          |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD11 | 6        | 0.12          |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD12 | 6        | 0.12          |
| (1,2569) | 1:105:B:ALA:HA   | 1:109:B:LEU:HD13 | 6        | 0.12          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD11 | 10       | 0.12          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD12 | 10       | 0.12          |
| (1,2557) | 1:102:B:ASN:HB2  | 1:157:B:LEU:HD13 | 10       | 0.12          |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG21 | 2        | 0.12          |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG22 | 2        | 0.12          |
| (1,2543) | 1:100:B:ASP:HA   | 1:162:B:THR:HG23 | 2        | 0.12          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 9        | 0.12          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 9        | 0.12          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 9        | 0.12          |
| (1,2537) | 1:99:B:LEU:HD11  | 1:111:B:VAL:HB   | 10       | 0.12          |
| (1,2537) | 1:99:B:LEU:HD12  | 1:111:B:VAL:HB   | 10       | 0.12          |
| (1,2537) | 1:99:B:LEU:HD13  | 1:111:B:VAL:HB   | 10       | 0.12          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG11 | 8        | 0.12          |
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG12 | 8        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2521) | 1:99:B:LEU:HD21  | 1:111:B:VAL:HG13 | 8        | 0.12          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG11 | 8        | 0.12          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG12 | 8        | 0.12          |
| (1,2521) | 1:99:B:LEU:HD22  | 1:111:B:VAL:HG13 | 8        | 0.12          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG11 | 8        | 0.12          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG12 | 8        | 0.12          |
| (1,2521) | 1:99:B:LEU:HD23  | 1:111:B:VAL:HG13 | 8        | 0.12          |
| (1,2493) | 1:99:B:LEU:HB2   | 1:109:B:LEU:HD21 | 6        | 0.12          |
| (1,2493) | 1:99:B:LEU:HB2   | 1:109:B:LEU:HD22 | 6        | 0.12          |
| (1,2493) | 1:99:B:LEU:HB2   | 1:109:B:LEU:HD23 | 6        | 0.12          |
| (1,2442) | 1:97:B:VAL:HG21  | 1:166:B:GLU:HA   | 7        | 0.12          |
| (1,2442) | 1:97:B:VAL:HG22  | 1:166:B:GLU:HA   | 7        | 0.12          |
| (1,2442) | 1:97:B:VAL:HG23  | 1:166:B:GLU:HA   | 7        | 0.12          |
| (1,2381) | 1:96:B:ARG:HB3   | 1:164:B:THR:HG21 | 3        | 0.12          |
| (1,2381) | 1:96:B:ARG:HB3   | 1:164:B:THR:HG22 | 3        | 0.12          |
| (1,2381) | 1:96:B:ARG:HB3   | 1:164:B:THR:HG23 | 3        | 0.12          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 6        | 0.12          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 6        | 0.12          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 6        | 0.12          |
| (1,2360) | 1:96:B:ARG:HA    | 1:96:B:ARG:HG3   | 8        | 0.12          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG11 | 5        | 0.12          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG12 | 5        | 0.12          |
| (1,2343) | 1:95:B:TRP:HB2   | 1:148:B:VAL:HG13 | 5        | 0.12          |
| (1,2330) | 1:94:B:ARG:HD3   | 1:168:B:PRO:HA   | 7        | 0.12          |
| (1,2323) | 1:94:B:ARG:HB3   | 1:168:B:PRO:HA   | 2        | 0.12          |
| (1,2291) | 1:91:B:THR:HA    | 1:91:B:THR:HB    | 2        | 0.12          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 2        | 0.12          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 2        | 0.12          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 2        | 0.12          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 6        | 0.12          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 6        | 0.12          |
| (1,2230) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 6        | 0.12          |
| (1,2225) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 9        | 0.12          |
| (1,2225) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 9        | 0.12          |
| (1,2225) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 9        | 0.12          |
| (1,2159) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB2  | 2        | 0.12          |
| (1,2157) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 1        | 0.12          |
| (1,2155) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD1  | 1        | 0.12          |
| (1,2155) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD2  | 1        | 0.12          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 2        | 0.12          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 2        | 0.12          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 2        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG21 | 6        | 0.12          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG22 | 6        | 0.12          |
| (1,2098) | 1:135:B:SER:HB2  | 1:139:A:THR:HG23 | 6        | 0.12          |
| (1,2093) | 1:134:A:ILE:HD11 | 1:140:B:ARG:HD2  | 9        | 0.12          |
| (1,2093) | 1:134:A:ILE:HD12 | 1:140:B:ARG:HD2  | 9        | 0.12          |
| (1,2093) | 1:134:A:ILE:HD13 | 1:140:B:ARG:HD2  | 9        | 0.12          |
| (1,2027) | 1:132:B:GLY:HA2  | 1:142:A:TYR:HB2  | 2        | 0.12          |
| (1,2025) | 1:132:B:GLY:HA2  | 1:140:A:ARG:HA   | 1        | 0.12          |
| (1,2023) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD1  | 1        | 0.12          |
| (1,2023) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD2  | 1        | 0.12          |
| (1,2010) | 1:171:A:LYS:H    | 1:172:A:LEU:HA   | 5        | 0.12          |
| (1,2000) | 1:169:A:MET:H    | 1:169:A:MET:HG3  | 3        | 0.12          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG11 | 10       | 0.12          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG12 | 10       | 0.12          |
| (1,1953) | 1:165:A:VAL:H    | 1:153:A:VAL:HG13 | 10       | 0.12          |
| (1,1925) | 1:162:A:THR:H    | 1:160:A:GLU:HG3  | 1        | 0.12          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG21 | 10       | 0.12          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG22 | 10       | 0.12          |
| (1,1914) | 1:161:A:GLY:H    | 1:162:A:THR:HG23 | 10       | 0.12          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 1        | 0.12          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 5        | 0.12          |
| (1,1911) | 1:161:A:GLY:H    | 1:161:A:GLY:HA2  | 6        | 0.12          |
| (1,1900) | 1:160:A:GLU:H    | 1:162:A:THR:HB   | 4        | 0.12          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG21 | 5        | 0.12          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG22 | 5        | 0.12          |
| (1,1887) | 1:158:A:SER:H    | 1:162:A:THR:HG23 | 5        | 0.12          |
| (1,1870) | 1:157:A:LEU:H    | 1:157:A:LEU:HB3  | 10       | 0.12          |
| (1,1849) | 1:155:A:SER:H    | 1:156:A:SER:HA   | 4        | 0.12          |
| (1,1844) | 1:154:A:SER:H    | 1:168:A:PRO:HD2  | 10       | 0.12          |
| (1,1804) | 1:152:A:GLN:HE21 | 1:169:A:MET:HA   | 6        | 0.12          |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB1  | 6        | 0.12          |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB2  | 6        | 0.12          |
| (1,1801) | 1:152:A:GLN:HE21 | 1:167:A:ALA:HB3  | 6        | 0.12          |
| (1,1766) | 1:149:A:ASP:H    | 1:169:A:MET:HG3  | 9        | 0.12          |
| (1,1743) | 1:148:A:VAL:H    | 1:146:A:PRO:HB3  | 4        | 0.12          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 7        | 0.12          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 7        | 0.12          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 7        | 0.12          |
| (1,1656) | 1:134:A:ILE:H    | 1:127:A:ARG:HG3  | 7        | 0.12          |
| (1,1655) | 1:134:A:ILE:H    | 1:127:A:ARG:HG2  | 9        | 0.12          |
| (1,1647) | 1:132:A:GLY:H    | 1:131:A:HIS:HB3  | 8        | 0.12          |
| (1,1642) | 1:132:A:GLY:H    | 1:129:A:ASP:HB2  | 1        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1627) | 1:129:A:ASP:H    | 1:132:A:GLY:H    | 2        | 0.12          |
| (1,1627) | 1:129:A:ASP:H    | 1:132:A:GLY:H    | 8        | 0.12          |
| (1,1624) | 1:129:A:ASP:H    | 1:131:A:HIS:HA   | 5        | 0.12          |
| (1,1598) | 1:128:A:GLN:H    | 1:127:A:ARG:HG2  | 9        | 0.12          |
| (1,1588) | 1:126:A:GLU:H    | 1:125:A:GLU:HG3  | 3        | 0.12          |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD21 | 2        | 0.12          |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD22 | 2        | 0.12          |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD23 | 2        | 0.12          |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 6        | 0.12          |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG21 | 1        | 0.12          |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG22 | 1        | 0.12          |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG23 | 1        | 0.12          |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG21 | 2        | 0.12          |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG22 | 2        | 0.12          |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG23 | 2        | 0.12          |
| (1,1545) | 1:120:A:ILE:H    | 1:140:A:ARG:HG3  | 1        | 0.12          |
| (1,1517) | 1:118:A:VAL:H    | 1:142:A:TYR:HB2  | 3        | 0.12          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG21 | 2        | 0.12          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG22 | 2        | 0.12          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG23 | 2        | 0.12          |
| (1,1478) | 1:114:A:LYS:H    | 1:112:A:LYS:HD3  | 5        | 0.12          |
| (1,1445) | 1:111:A:VAL:H    | 1:110:A:THR:HB   | 9        | 0.12          |
| (1,1432) | 1:109:A:LEU:H    | 1:157:A:LEU:HD11 | 2        | 0.12          |
| (1,1432) | 1:109:A:LEU:H    | 1:157:A:LEU:HD12 | 2        | 0.12          |
| (1,1432) | 1:109:A:LEU:H    | 1:157:A:LEU:HD13 | 2        | 0.12          |
| (1,1428) | 1:109:A:LEU:H    | 1:109:A:LEU:HB3  | 4        | 0.12          |
| (1,1382) | 1:102:A:ASN:HD22 | 1:161:A:GLY:HA2  | 10       | 0.12          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG21 | 2        | 0.12          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG22 | 2        | 0.12          |
| (1,1357) | 1:99:A:LEU:H     | 1:101:A:VAL:HG23 | 2        | 0.12          |
| (1,1345) | 1:97:A:VAL:H     | 1:165:A:VAL:H    | 1        | 0.12          |
| (1,1327) | 1:94:A:ARG:H     | 1:169:A:MET:HG2  | 10       | 0.12          |
| (1,1311) | 1:170:A:PRO:HB2  | 1:170:A:PRO:HG2  | 7        | 0.12          |
| (1,1287) | 1:169:A:MET:HA   | 1:169:A:MET:HB3  | 10       | 0.12          |
| (1,1280) | 1:168:A:PRO:HB2  | 1:170:A:PRO:HD3  | 9        | 0.12          |
| (1,1277) | 1:168:A:PRO:HA   | 1:169:A:MET:HG3  | 8        | 0.12          |
| (1,1193) | 1:158:A:SER:HB3  | 1:160:A:GLU:HB3  | 7        | 0.12          |
| (1,1173) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB3  | 2        | 0.12          |
| (1,1173) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB3  | 2        | 0.12          |
| (1,1173) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB3  | 2        | 0.12          |
| (1,1172) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB2  | 4        | 0.12          |
| (1,1172) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB2  | 4        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1172) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB2  | 4        | 0.12          |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 4        | 0.12          |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 9        | 0.12          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD11 | 3        | 0.12          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD12 | 3        | 0.12          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD13 | 3        | 0.12          |
| (1,1139) | 1:156:A:SER:HB3  | 1:157:A:LEU:HB3  | 3        | 0.12          |
| (1,1079) | 1:153:A:VAL:HB   | 1:154:A:SER:HA   | 5        | 0.12          |
| (1,1079) | 1:153:A:VAL:HB   | 1:154:A:SER:HA   | 8        | 0.12          |
| (1,1036) | 1:150:A:PRO:HA   | 1:151:A:THR:HG21 | 4        | 0.12          |
| (1,1036) | 1:150:A:PRO:HA   | 1:151:A:THR:HG22 | 4        | 0.12          |
| (1,1036) | 1:150:A:PRO:HA   | 1:151:A:THR:HG23 | 4        | 0.12          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 4        | 0.12          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 4        | 0.12          |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 4        | 0.12          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG11 | 4        | 0.12          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG12 | 4        | 0.12          |
| (1,912)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG13 | 4        | 0.12          |
| (1,849)  | 1:141:A:LYS:HB2  | 1:141:A:LYS:HE2  | 7        | 0.12          |
| (1,782)  | 1:131:A:HIS:HB2  | 1:132:A:GLY:HA2  | 10       | 0.12          |
| (1,766)  | 1:129:A:ASP:HA   | 1:130:A:GLU:HB2  | 10       | 0.12          |
| (1,764)  | 1:129:A:ASP:HA   | 1:129:A:ASP:HB3  | 4        | 0.12          |
| (1,719)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD1  | 10       | 0.12          |
| (1,719)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD2  | 10       | 0.12          |
| (1,718)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HB3  | 9        | 0.12          |
| (1,712)  | 1:126:A:GLU:HB3  | 1:133:A:TYR:HB2  | 10       | 0.12          |
| (1,695)  | 1:123:A:LYS:HD3  | 1:137:A:CYS:HB2  | 4        | 0.12          |
| (1,680)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HG3  | 5        | 0.12          |
| (1,652)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HB2  | 2        | 0.12          |
| (1,652)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HB2  | 2        | 0.12          |
| (1,652)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HB2  | 2        | 0.12          |
| (1,647)  | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 7        | 0.12          |
| (1,647)  | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 7        | 0.12          |
| (1,647)  | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 7        | 0.12          |
| (1,608)  | 1:119:A:GLU:HA   | 1:141:A:LYS:HA   | 5        | 0.12          |
| (1,577)  | 1:118:A:VAL:HB   | 1:153:A:VAL:HG21 | 4        | 0.12          |
| (1,577)  | 1:118:A:VAL:HB   | 1:153:A:VAL:HG22 | 4        | 0.12          |
| (1,577)  | 1:118:A:VAL:HB   | 1:153:A:VAL:HG23 | 4        | 0.12          |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD21 | 3        | 0.12          |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD22 | 3        | 0.12          |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD23 | 3        | 0.12          |
| (1,551)  | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 2        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 2        | 0.12          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 2        | 0.12          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG21 | 1        | 0.12          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG22 | 1        | 0.12          |
| (1,546) | 1:117:A:VAL:HA   | 1:143:A:THR:HG23 | 1        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 1        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 1        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 1        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 4        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 4        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 4        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG21 | 7        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG22 | 7        | 0.12          |
| (1,521) | 1:116:A:GLY:HA2  | 1:118:A:VAL:HG23 | 7        | 0.12          |
| (1,517) | 1:115:A:ASP:HB3  | 1:150:A:PRO:HG2  | 9        | 0.12          |
| (1,509) | 1:114:A:LYS:HA   | 1:114:A:LYS:HB2  | 6        | 0.12          |
| (1,502) | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 2        | 0.12          |
| (1,502) | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 2        | 0.12          |
| (1,502) | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 2        | 0.12          |
| (1,502) | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 9        | 0.12          |
| (1,502) | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 9        | 0.12          |
| (1,502) | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 9        | 0.12          |
| (1,419) | 1:111:A:VAL:HA   | 1:120:A:ILE:HG13 | 6        | 0.12          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD11 | 3        | 0.12          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD12 | 3        | 0.12          |
| (1,364) | 1:109:A:LEU:HG   | 1:120:A:ILE:HD13 | 3        | 0.12          |
| (1,359) | 1:109:A:LEU:HB2  | 1:122:A:GLY:HA2  | 8        | 0.12          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 7        | 0.12          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 7        | 0.12          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 7        | 0.12          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 3        | 0.12          |
| (1,283) | 1:105:A:ALA:HA   | 1:106:A:PRO:HB3  | 10       | 0.12          |
| (1,280) | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA3  | 4        | 0.12          |
| (1,280) | 1:102:A:ASN:HB3  | 1:161:A:GLY:HA3  | 6        | 0.12          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG21 | 4        | 0.12          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG22 | 4        | 0.12          |
| (1,262) | 1:100:A:ASP:HA   | 1:162:A:THR:HG23 | 4        | 0.12          |
| (1,253) | 1:99:A:LEU:HD21  | 1:142:A:TYR:HD1  | 10       | 0.12          |
| (1,253) | 1:99:A:LEU:HD21  | 1:142:A:TYR:HD2  | 10       | 0.12          |
| (1,253) | 1:99:A:LEU:HD22  | 1:142:A:TYR:HD1  | 10       | 0.12          |
| (1,253) | 1:99:A:LEU:HD22  | 1:142:A:TYR:HD2  | 10       | 0.12          |
| (1,253) | 1:99:A:LEU:HD23  | 1:142:A:TYR:HD1  | 10       | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,253)  | 1:99:A:LEU:HD23 | 1:142:A:TYR:HD2  | 10       | 0.12          |
| (1,229)  | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG11 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG12 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD11 | 1:111:A:VAL:HG13 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG11 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG12 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD12 | 1:111:A:VAL:HG13 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG11 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG12 | 5        | 0.12          |
| (1,229)  | 1:99:A:LEU:HD13 | 1:111:A:VAL:HG13 | 5        | 0.12          |
| (1,226)  | 1:99:A:LEU:HD11 | 1:101:A:VAL:HG21 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD11 | 1:101:A:VAL:HG22 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD11 | 1:101:A:VAL:HG23 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG21 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG22 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD12 | 1:101:A:VAL:HG23 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG21 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG22 | 10       | 0.12          |
| (1,226)  | 1:99:A:LEU:HD13 | 1:101:A:VAL:HG23 | 10       | 0.12          |
| (1,216)  | 1:99:A:LEU:HB3  | 1:109:A:LEU:HD11 | 2        | 0.12          |
| (1,216)  | 1:99:A:LEU:HB3  | 1:109:A:LEU:HD12 | 2        | 0.12          |
| (1,216)  | 1:99:A:LEU:HB3  | 1:109:A:LEU:HD13 | 2        | 0.12          |
| (1,161)  | 1:97:A:VAL:HG21 | 1:166:A:GLU:HA   | 10       | 0.12          |
| (1,161)  | 1:97:A:VAL:HG22 | 1:166:A:GLU:HA   | 10       | 0.12          |
| (1,161)  | 1:97:A:VAL:HG23 | 1:166:A:GLU:HA   | 10       | 0.12          |
| (1,141)  | 1:97:A:VAL:HG11 | 1:142:A:TYR:HD1  | 7        | 0.12          |
| (1,141)  | 1:97:A:VAL:HG11 | 1:142:A:TYR:HD2  | 7        | 0.12          |
| (1,141)  | 1:97:A:VAL:HG12 | 1:142:A:TYR:HD1  | 7        | 0.12          |
| (1,141)  | 1:97:A:VAL:HG12 | 1:142:A:TYR:HD2  | 7        | 0.12          |
| (1,141)  | 1:97:A:VAL:HG13 | 1:142:A:TYR:HD1  | 7        | 0.12          |
| (1,141)  | 1:97:A:VAL:HG13 | 1:142:A:TYR:HD2  | 7        | 0.12          |
| (1,69)   | 1:95:A:TRP:HB3  | 1:166:A:GLU:HB2  | 1        | 0.12          |
| (1,45)   | 1:94:A:ARG:HG2  | 1:168:A:PRO:HB2  | 4        | 0.12          |
| (1,35)   | 1:94:A:ARG:HB2  | 1:94:A:ARG:HG3   | 8        | 0.12          |
| (1,29)   | 1:94:A:ARG:HA   | 1:168:A:PRO:HA   | 10       | 0.12          |
| (1,23)   | 1:94:A:ARG:HA   | 1:94:A:ARG:HB3   | 9        | 0.12          |
| (1,4263) | 1:167:B:ALA:H   | 1:166:B:GLU:HB3  | 1        | 0.11          |
| (1,4197) | 1:162:B:THR:H   | 1:102:B:ASN:HB3  | 1        | 0.11          |
| (1,4192) | 1:161:B:GLY:H   | 1:161:B:GLY:HA2  | 1        | 0.11          |
| (1,4192) | 1:161:B:GLY:H   | 1:161:B:GLY:HA2  | 3        | 0.11          |
| (1,4192) | 1:161:B:GLY:H   | 1:161:B:GLY:HA2  | 9        | 0.11          |
| (1,4182) | 1:161:B:GLY:H   | 1:102:B:ASN:HB2  | 8        | 0.11          |

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| Key      | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|----------|---------------|------------------|----------|---------------|
| (1,4128) | 1:155:B:SER:H | 1:154:B:SER:HB2  | 2        | 0.11          |
| (1,4124) | 1:154:B:SER:H | 1:167:B:ALA:HB1  | 6        | 0.11          |
| (1,4124) | 1:154:B:SER:H | 1:167:B:ALA:HB2  | 6        | 0.11          |
| (1,4124) | 1:154:B:SER:H | 1:167:B:ALA:HB3  | 6        | 0.11          |
| (1,4044) | 1:149:B:ASP:H | 1:152:B:GLN:HB3  | 7        | 0.11          |
| (1,4043) | 1:149:B:ASP:H | 1:152:B:GLN:HB2  | 5        | 0.11          |
| (1,4034) | 1:148:B:VAL:H | 1:149:B:ASP:H    | 3        | 0.11          |
| (1,4034) | 1:148:B:VAL:H | 1:149:B:ASP:H    | 10       | 0.11          |
| (1,3963) | 1:137:B:CYS:H | 1:138:B:PHE:HE1  | 4        | 0.11          |
| (1,3963) | 1:137:B:CYS:H | 1:138:B:PHE:HE2  | 4        | 0.11          |
| (1,3936) | 1:134:B:ILE:H | 1:127:B:ARG:HG2  | 7        | 0.11          |
| (1,3936) | 1:134:B:ILE:H | 1:127:B:ARG:HG2  | 10       | 0.11          |
| (1,3928) | 1:132:B:GLY:H | 1:131:B:HIS:HB3  | 3        | 0.11          |
| (1,3919) | 1:131:B:HIS:H | 1:132:B:GLY:HA3  | 2        | 0.11          |
| (1,3879) | 1:128:B:GLN:H | 1:127:B:ARG:HG2  | 2        | 0.11          |
| (1,3869) | 1:126:B:GLU:H | 1:125:B:GLU:HG3  | 2        | 0.11          |
| (1,3866) | 1:126:B:GLU:H | 1:125:B:GLU:HA   | 5        | 0.11          |
| (1,3850) | 1:123:B:LYS:H | 1:109:B:LEU:HD21 | 7        | 0.11          |
| (1,3850) | 1:123:B:LYS:H | 1:109:B:LEU:HD22 | 7        | 0.11          |
| (1,3850) | 1:123:B:LYS:H | 1:109:B:LEU:HD23 | 7        | 0.11          |
| (1,3844) | 1:123:B:LYS:H | 1:105:B:ALA:HB1  | 2        | 0.11          |
| (1,3844) | 1:123:B:LYS:H | 1:105:B:ALA:HB2  | 2        | 0.11          |
| (1,3844) | 1:123:B:LYS:H | 1:105:B:ALA:HB3  | 2        | 0.11          |
| (1,3837) | 1:121:B:THR:H | 1:121:B:THR:HG21 | 10       | 0.11          |
| (1,3837) | 1:121:B:THR:H | 1:121:B:THR:HG22 | 10       | 0.11          |
| (1,3837) | 1:121:B:THR:H | 1:121:B:THR:HG23 | 10       | 0.11          |
| (1,3821) | 1:120:B:ILE:H | 1:120:B:ILE:HD11 | 4        | 0.11          |
| (1,3821) | 1:120:B:ILE:H | 1:120:B:ILE:HD12 | 4        | 0.11          |
| (1,3821) | 1:120:B:ILE:H | 1:120:B:ILE:HD13 | 4        | 0.11          |
| (1,3805) | 1:119:B:GLU:H | 1:114:B:LYS:HB2  | 4        | 0.11          |
| (1,3790) | 1:117:B:VAL:H | 1:144:B:LEU:H    | 5        | 0.11          |
| (1,3790) | 1:117:B:VAL:H | 1:144:B:LEU:H    | 9        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG21 | 3        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG22 | 3        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG23 | 3        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG21 | 4        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG22 | 4        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG23 | 4        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG21 | 9        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG22 | 9        | 0.11          |
| (1,3787) | 1:117:B:VAL:H | 1:118:B:VAL:HG23 | 9        | 0.11          |
| (1,3726) | 1:111:B:VAL:H | 1:110:B:THR:HB   | 2        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3723) | 1:110:B:THR:H    | 1:122:B:GLY:H    | 5        | 0.11          |
| (1,3670) | 1:105:B:ALA:H    | 1:106:B:PRO:HD3  | 9        | 0.11          |
| (1,3643) | 1:101:B:VAL:H    | 1:120:B:ILE:HG21 | 9        | 0.11          |
| (1,3643) | 1:101:B:VAL:H    | 1:120:B:ILE:HG22 | 9        | 0.11          |
| (1,3643) | 1:101:B:VAL:H    | 1:120:B:ILE:HG23 | 9        | 0.11          |
| (1,3626) | 1:97:B:VAL:H     | 1:165:B:VAL:H    | 6        | 0.11          |
| (1,3592) | 1:170:B:PRO:HB2  | 1:170:B:PRO:HG2  | 2        | 0.11          |
| (1,3592) | 1:170:B:PRO:HB2  | 1:170:B:PRO:HG2  | 5        | 0.11          |
| (1,3592) | 1:170:B:PRO:HB2  | 1:170:B:PRO:HG2  | 6        | 0.11          |
| (1,3592) | 1:170:B:PRO:HB2  | 1:170:B:PRO:HG2  | 10       | 0.11          |
| (1,3568) | 1:169:B:MET:HA   | 1:169:B:MET:HB3  | 6        | 0.11          |
| (1,3563) | 1:168:B:PRO:HB3  | 1:169:B:MET:HA   | 2        | 0.11          |
| (1,3481) | 1:159:B:PRO:HA   | 1:159:B:PRO:HG3  | 4        | 0.11          |
| (1,3474) | 1:158:B:SER:HB3  | 1:160:B:GLU:HB3  | 5        | 0.11          |
| (1,3455) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HG   | 7        | 0.11          |
| (1,3455) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HG   | 7        | 0.11          |
| (1,3455) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HG   | 7        | 0.11          |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 5        | 0.11          |
| (1,3395) | 1:155:B:SER:HB2  | 1:163:B:LEU:HA   | 9        | 0.11          |
| (1,3391) | 1:155:B:SER:HA   | 1:165:B:VAL:HA   | 5        | 0.11          |
| (1,3391) | 1:155:B:SER:HA   | 1:165:B:VAL:HA   | 10       | 0.11          |
| (1,3345) | 1:152:B:GLN:HB2  | 1:168:B:PRO:HD3  | 9        | 0.11          |
| (1,3292) | 1:148:B:VAL:HG11 | 1:169:B:MET:HA   | 3        | 0.11          |
| (1,3292) | 1:148:B:VAL:HG12 | 1:169:B:MET:HA   | 3        | 0.11          |
| (1,3292) | 1:148:B:VAL:HG13 | 1:169:B:MET:HA   | 3        | 0.11          |
| (1,3292) | 1:148:B:VAL:HG11 | 1:169:B:MET:HA   | 10       | 0.11          |
| (1,3292) | 1:148:B:VAL:HG12 | 1:169:B:MET:HA   | 10       | 0.11          |
| (1,3292) | 1:148:B:VAL:HG13 | 1:169:B:MET:HA   | 10       | 0.11          |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 1        | 0.11          |
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 1        | 0.11          |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 1        | 0.11          |
| (1,3288) | 1:148:B:VAL:HG11 | 1:153:B:VAL:HA   | 6        | 0.11          |
| (1,3288) | 1:148:B:VAL:HG12 | 1:153:B:VAL:HA   | 6        | 0.11          |
| (1,3288) | 1:148:B:VAL:HG13 | 1:153:B:VAL:HA   | 6        | 0.11          |
| (1,3266) | 1:148:B:VAL:HA   | 1:149:B:ASP:HB3  | 3        | 0.11          |
| (1,3249) | 1:146:B:PRO:HB3  | 1:147:B:GLY:HA3  | 2        | 0.11          |
| (1,3242) | 1:145:B:PRO:HD2  | 1:146:B:PRO:HB2  | 4        | 0.11          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG21 | 9        | 0.11          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG22 | 9        | 0.11          |
| (1,3194) | 1:144:B:LEU:HB2  | 1:148:B:VAL:HG23 | 9        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD21 | 4        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD22 | 4        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD23 | 4        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD21 | 4        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD22 | 4        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD23 | 4        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD21 | 9        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD22 | 9        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD23 | 9        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD21 | 9        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD22 | 9        | 0.11          |
| (1,3162) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD23 | 9        | 0.11          |
| (1,3161) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD11 | 3        | 0.11          |
| (1,3161) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD12 | 3        | 0.11          |
| (1,3161) | 1:142:B:TYR:HD1  | 1:144:B:LEU:HD13 | 3        | 0.11          |
| (1,3161) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD11 | 3        | 0.11          |
| (1,3161) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD12 | 3        | 0.11          |
| (1,3161) | 1:142:B:TYR:HD2  | 1:144:B:LEU:HD13 | 3        | 0.11          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE1  | 7        | 0.11          |
| (1,3030) | 1:128:B:GLN:HA   | 1:133:B:TYR:HE2  | 7        | 0.11          |
| (1,3015) | 1:127:B:ARG:HA   | 1:127:B:ARG:HB3  | 2        | 0.11          |
| (1,3013) | 1:126:B:GLU:HG3  | 1:134:B:ILE:HG23 | 1        | 0.11          |
| (1,2977) | 1:123:B:LYS:HD2  | 1:137:B:CYS:HB3  | 3        | 0.11          |
| (1,2977) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB3  | 4        | 0.11          |
| (1,2963) | 1:123:B:LYS:HA   | 1:123:B:LYS:HE3  | 10       | 0.11          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 5        | 0.11          |
| (1,2961) | 1:123:B:LYS:HA   | 1:123:B:LYS:HG3  | 7        | 0.11          |
| (1,2933) | 1:120:B:ILE:HD11 | 1:140:B:ARG:HB2  | 9        | 0.11          |
| (1,2933) | 1:120:B:ILE:HD12 | 1:140:B:ARG:HB2  | 9        | 0.11          |
| (1,2933) | 1:120:B:ILE:HD13 | 1:140:B:ARG:HB2  | 9        | 0.11          |
| (1,2920) | 1:120:B:ILE:HG12 | 1:121:B:THR:HA   | 6        | 0.11          |
| (1,2914) | 1:120:B:ILE:HB   | 1:120:B:ILE:HD11 | 4        | 0.11          |
| (1,2914) | 1:120:B:ILE:HB   | 1:120:B:ILE:HD12 | 4        | 0.11          |
| (1,2914) | 1:120:B:ILE:HB   | 1:120:B:ILE:HD13 | 4        | 0.11          |
| (1,2886) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG13 | 8        | 0.11          |
| (1,2885) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG12 | 2        | 0.11          |
| (1,2864) | 1:118:B:VAL:HG11 | 1:142:B:TYR:HB2  | 6        | 0.11          |
| (1,2864) | 1:118:B:VAL:HG12 | 1:142:B:TYR:HB2  | 6        | 0.11          |
| (1,2864) | 1:118:B:VAL:HG13 | 1:142:B:TYR:HB2  | 6        | 0.11          |
| (1,2831) | 1:117:B:VAL:HA   | 1:148:B:VAL:HB   | 5        | 0.11          |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG21 | 8        | 0.11          |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG22 | 8        | 0.11          |
| (1,2794) | 1:115:B:ASP:HB2  | 1:117:B:VAL:HG23 | 8        | 0.11          |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 2        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 2        | 0.11          |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 2        | 0.11          |
| (1,2783) | 1:113:B:THR:HG21 | 1:150:B:PRO:HB3  | 10       | 0.11          |
| (1,2783) | 1:113:B:THR:HG22 | 1:150:B:PRO:HB3  | 10       | 0.11          |
| (1,2783) | 1:113:B:THR:HG23 | 1:150:B:PRO:HB3  | 10       | 0.11          |
| (1,2749) | 1:112:B:LYS:HG2  | 1:121:B:THR:HB   | 9        | 0.11          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG21 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG22 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG11 | 1:118:B:VAL:HG23 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG21 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG22 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG12 | 1:118:B:VAL:HG23 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG21 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG22 | 10       | 0.11          |
| (1,2713) | 1:111:B:VAL:HG13 | 1:118:B:VAL:HG23 | 10       | 0.11          |
| (1,2708) | 1:111:B:VAL:HG11 | 1:112:B:LYS:HE2  | 6        | 0.11          |
| (1,2708) | 1:111:B:VAL:HG12 | 1:112:B:LYS:HE2  | 6        | 0.11          |
| (1,2708) | 1:111:B:VAL:HG13 | 1:112:B:LYS:HE2  | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD21 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD22 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD11 | 1:157:B:LEU:HD23 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD21 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD22 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD12 | 1:157:B:LEU:HD23 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD21 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD22 | 6        | 0.11          |
| (1,2652) | 1:109:B:LEU:HD13 | 1:157:B:LEU:HD23 | 6        | 0.11          |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD21 | 1        | 0.11          |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD22 | 1        | 0.11          |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD23 | 1        | 0.11          |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD21 | 10       | 0.11          |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD22 | 10       | 0.11          |
| (1,2647) | 1:109:B:LEU:HG   | 1:157:B:LEU:HD23 | 10       | 0.11          |
| (1,2643) | 1:109:B:LEU:HB3  | 1:121:B:THR:HB   | 8        | 0.11          |
| (1,2629) | 1:108:B:GLU:HG3  | 1:123:B:LYS:HE3  | 8        | 0.11          |
| (1,2617) | 1:108:B:GLU:HA   | 1:108:B:GLU:HG2  | 10       | 0.11          |
| (1,2583) | 1:105:B:ALA:HB1  | 1:123:B:LYS:HA   | 3        | 0.11          |
| (1,2583) | 1:105:B:ALA:HB2  | 1:123:B:LYS:HA   | 3        | 0.11          |
| (1,2583) | 1:105:B:ALA:HB3  | 1:123:B:LYS:HA   | 3        | 0.11          |
| (1,2578) | 1:105:B:ALA:HB1  | 1:107:B:ASP:HB3  | 5        | 0.11          |
| (1,2578) | 1:105:B:ALA:HB2  | 1:107:B:ASP:HB3  | 5        | 0.11          |
| (1,2578) | 1:105:B:ALA:HB3  | 1:107:B:ASP:HB3  | 5        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2568) | 1:105:B:ALA:HA   | 1:108:B:GLU:HB3  | 1        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG21 | 1:157:B:LEU:HD21 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG21 | 1:157:B:LEU:HD22 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG21 | 1:157:B:LEU:HD23 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG22 | 1:157:B:LEU:HD21 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG22 | 1:157:B:LEU:HD22 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG22 | 1:157:B:LEU:HD23 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG23 | 1:157:B:LEU:HD21 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG23 | 1:157:B:LEU:HD22 | 3        | 0.11          |
| (1,2554) | 1:101:B:VAL:HG23 | 1:157:B:LEU:HD23 | 3        | 0.11          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD11 | 7        | 0.11          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD12 | 7        | 0.11          |
| (1,2497) | 1:99:B:LEU:HB3   | 1:109:B:LEU:HD13 | 7        | 0.11          |
| (1,2457) | 1:98:B:SER:HA    | 1:162:B:THR:HG21 | 9        | 0.11          |
| (1,2457) | 1:98:B:SER:HA    | 1:162:B:THR:HG22 | 9        | 0.11          |
| (1,2457) | 1:98:B:SER:HA    | 1:162:B:THR:HG23 | 9        | 0.11          |
| (1,2442) | 1:97:B:VAL:HG21  | 1:166:B:GLU:HA   | 4        | 0.11          |
| (1,2442) | 1:97:B:VAL:HG22  | 1:166:B:GLU:HA   | 4        | 0.11          |
| (1,2442) | 1:97:B:VAL:HG23  | 1:166:B:GLU:HA   | 4        | 0.11          |
| (1,2442) | 1:97:B:VAL:HG21  | 1:166:B:GLU:HA   | 8        | 0.11          |
| (1,2442) | 1:97:B:VAL:HG22  | 1:166:B:GLU:HA   | 8        | 0.11          |
| (1,2442) | 1:97:B:VAL:HG23  | 1:166:B:GLU:HA   | 8        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD1  | 1        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD2  | 1        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD1  | 1        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD2  | 1        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD1  | 1        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD2  | 1        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD1  | 3        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG11  | 1:142:B:TYR:HD2  | 3        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD1  | 3        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG12  | 1:142:B:TYR:HD2  | 3        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD1  | 3        | 0.11          |
| (1,2422) | 1:97:B:VAL:HG13  | 1:142:B:TYR:HD2  | 3        | 0.11          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG21 | 6        | 0.11          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG22 | 6        | 0.11          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG23 | 6        | 0.11          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG21 | 9        | 0.11          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG22 | 9        | 0.11          |
| (1,2413) | 1:97:B:VAL:HB    | 1:165:B:VAL:HG23 | 9        | 0.11          |
| (1,2388) | 1:96:B:ARG:HG2   | 1:166:B:GLU:HG2  | 8        | 0.11          |
| (1,2382) | 1:96:B:ARG:HB3   | 1:166:B:GLU:HA   | 5        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 4        | 0.11          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 4        | 0.11          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 4        | 0.11          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG21 | 7        | 0.11          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG22 | 7        | 0.11          |
| (1,2369) | 1:96:B:ARG:HA    | 1:165:B:VAL:HG23 | 7        | 0.11          |
| (1,2352) | 1:95:B:TRP:HB2   | 1:168:B:PRO:HB2  | 3        | 0.11          |
| (1,2291) | 1:91:B:THR:HA    | 1:91:B:THR:HB    | 8        | 0.11          |
| (1,2244) | 1:136:B:ARG:HG2  | 1:138:A:PHE:HA   | 8        | 0.11          |
| (1,2218) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 2        | 0.11          |
| (1,2218) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 2        | 0.11          |
| (1,2218) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 2        | 0.11          |
| (1,2213) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 7        | 0.11          |
| (1,2155) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD1  | 2        | 0.11          |
| (1,2155) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD2  | 2        | 0.11          |
| (1,2112) | 1:136:B:ARG:HG2  | 1:138:A:PHE:HA   | 8        | 0.11          |
| (1,2086) | 1:134:A:ILE:HG21 | 1:138:B:PHE:HB3  | 2        | 0.11          |
| (1,2086) | 1:134:A:ILE:HG22 | 1:138:B:PHE:HB3  | 2        | 0.11          |
| (1,2086) | 1:134:A:ILE:HG23 | 1:138:B:PHE:HB3  | 2        | 0.11          |
| (1,2081) | 1:134:A:ILE:HA   | 1:140:B:ARG:HD3  | 7        | 0.11          |
| (1,2023) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD1  | 2        | 0.11          |
| (1,2023) | 1:131:A:HIS:HB2  | 1:142:B:TYR:HD2  | 2        | 0.11          |
| (1,1982) | 1:167:A:ALA:H    | 1:166:A:GLU:HB3  | 10       | 0.11          |
| (1,1958) | 1:165:A:VAL:H    | 1:166:A:GLU:HB3  | 7        | 0.11          |
| (1,1909) | 1:161:A:GLY:H    | 1:160:A:GLU:HB3  | 2        | 0.11          |
| (1,1888) | 1:158:A:SER:H    | 1:162:A:THR:H    | 1        | 0.11          |
| (1,1870) | 1:157:A:LEU:H    | 1:157:A:LEU:HB3  | 9        | 0.11          |
| (1,1849) | 1:155:A:SER:H    | 1:156:A:SER:HA   | 3        | 0.11          |
| (1,1816) | 1:153:A:VAL:H    | 1:149:A:ASP:HB2  | 7        | 0.11          |
| (1,1803) | 1:152:A:GLN:HE21 | 1:168:A:PRO:HD2  | 4        | 0.11          |
| (1,1784) | 1:152:A:GLN:H    | 1:149:A:ASP:HB3  | 6        | 0.11          |
| (1,1762) | 1:149:A:ASP:H    | 1:152:A:GLN:HB2  | 7        | 0.11          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 2        | 0.11          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 2        | 0.11          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 2        | 0.11          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG11 | 7        | 0.11          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG12 | 7        | 0.11          |
| (1,1730) | 1:144:A:LEU:H    | 1:148:A:VAL:HG13 | 7        | 0.11          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 1        | 0.11          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 1        | 0.11          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 1        | 0.11          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 2        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 2        | 0.11          |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 2        | 0.11          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD11  | 7        | 0.11          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD12  | 7        | 0.11          |
| (1,1690) | 1:140:A:ARG:H    | 1:99:A:LEU:HD13  | 7        | 0.11          |
| (1,1668) | 1:135:A:SER:H    | 1:135:A:SER:HB3  | 5        | 0.11          |
| (1,1657) | 1:134:A:ILE:H    | 1:133:A:TYR:HB3  | 8        | 0.11          |
| (1,1643) | 1:132:A:GLY:H    | 1:130:A:GLU:HB3  | 9        | 0.11          |
| (1,1627) | 1:129:A:ASP:H    | 1:132:A:GLY:H    | 9        | 0.11          |
| (1,1622) | 1:129:A:ASP:H    | 1:129:A:ASP:HB3  | 8        | 0.11          |
| (1,1616) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HG2  | 3        | 0.11          |
| (1,1613) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HA   | 6        | 0.11          |
| (1,1611) | 1:128:A:GLN:HE22 | 1:128:A:GLN:H    | 1        | 0.11          |
| (1,1600) | 1:128:A:GLN:H    | 1:127:A:ARG:HD2  | 5        | 0.11          |
| (1,1598) | 1:128:A:GLN:H    | 1:127:A:ARG:HG2  | 6        | 0.11          |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD1  | 6        | 0.11          |
| (1,1596) | 1:127:A:ARG:H    | 1:133:A:TYR:HD2  | 6        | 0.11          |
| (1,1581) | 1:125:A:GLU:H    | 1:108:A:GLU:HG3  | 1        | 0.11          |
| (1,1580) | 1:125:A:GLU:H    | 1:108:A:GLU:HG2  | 8        | 0.11          |
| (1,1576) | 1:124:A:HIS:H    | 1:136:A:ARG:HA   | 1        | 0.11          |
| (1,1576) | 1:124:A:HIS:H    | 1:136:A:ARG:HA   | 8        | 0.11          |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD11 | 7        | 0.11          |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD12 | 7        | 0.11          |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD13 | 7        | 0.11          |
| (1,1567) | 1:123:A:LYS:H    | 1:109:A:LEU:HG   | 9        | 0.11          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB1  | 4        | 0.11          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB2  | 4        | 0.11          |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB3  | 4        | 0.11          |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG21 | 3        | 0.11          |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG22 | 3        | 0.11          |
| (1,1556) | 1:121:A:THR:H    | 1:121:A:THR:HG23 | 3        | 0.11          |
| (1,1546) | 1:120:A:ILE:H    | 1:142:A:TYR:H    | 9        | 0.11          |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD11 | 10       | 0.11          |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD12 | 10       | 0.11          |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD13 | 10       | 0.11          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG21 | 4        | 0.11          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG22 | 4        | 0.11          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG23 | 4        | 0.11          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG21 | 7        | 0.11          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG22 | 7        | 0.11          |
| (1,1506) | 1:117:A:VAL:H    | 1:118:A:VAL:HG23 | 7        | 0.11          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD11 | 8        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD12 | 8        | 0.11          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD13 | 8        | 0.11          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD11 | 10       | 0.11          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD12 | 10       | 0.11          |
| (1,1439) | 1:110:A:THR:H    | 1:120:A:ILE:HD13 | 10       | 0.11          |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD11 | 1        | 0.11          |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD12 | 1        | 0.11          |
| (1,1421) | 1:108:A:GLU:H    | 1:109:A:LEU:HD13 | 1        | 0.11          |
| (1,1391) | 1:105:A:ALA:H    | 1:108:A:GLU:HB3  | 2        | 0.11          |
| (1,1389) | 1:105:A:ALA:H    | 1:106:A:PRO:HD3  | 4        | 0.11          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD21 | 7        | 0.11          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD22 | 7        | 0.11          |
| (1,1384) | 1:103:A:HIS:H    | 1:109:A:LEU:HD23 | 7        | 0.11          |
| (1,1345) | 1:97:A:VAL:H     | 1:165:A:VAL:H    | 2        | 0.11          |
| (1,1311) | 1:170:A:PRO:HB2  | 1:170:A:PRO:HG2  | 5        | 0.11          |
| (1,1311) | 1:170:A:PRO:HB2  | 1:170:A:PRO:HG2  | 6        | 0.11          |
| (1,1311) | 1:170:A:PRO:HB2  | 1:170:A:PRO:HG2  | 8        | 0.11          |
| (1,1282) | 1:168:A:PRO:HB3  | 1:169:A:MET:HA   | 5        | 0.11          |
| (1,1282) | 1:168:A:PRO:HB3  | 1:169:A:MET:HA   | 10       | 0.11          |
| (1,1280) | 1:168:A:PRO:HB2  | 1:170:A:PRO:HD3  | 6        | 0.11          |
| (1,1276) | 1:168:A:PRO:HA   | 1:169:A:MET:HG2  | 1        | 0.11          |
| (1,1248) | 1:165:A:VAL:HG21 | 1:167:A:ALA:HA   | 2        | 0.11          |
| (1,1248) | 1:165:A:VAL:HG22 | 1:167:A:ALA:HA   | 2        | 0.11          |
| (1,1248) | 1:165:A:VAL:HG23 | 1:167:A:ALA:HA   | 2        | 0.11          |
| (1,1192) | 1:158:A:SER:HB2  | 1:162:A:THR:HB   | 8        | 0.11          |
| (1,1172) | 1:157:A:LEU:HD11 | 1:163:A:LEU:HB2  | 10       | 0.11          |
| (1,1172) | 1:157:A:LEU:HD12 | 1:163:A:LEU:HB2  | 10       | 0.11          |
| (1,1172) | 1:157:A:LEU:HD13 | 1:163:A:LEU:HB2  | 10       | 0.11          |
| (1,1155) | 1:157:A:LEU:HB2  | 1:163:A:LEU:HA   | 10       | 0.11          |
| (1,1149) | 1:157:A:LEU:HA   | 1:163:A:LEU:HB3  | 2        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD11 | 1        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD12 | 1        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD13 | 1        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD11 | 2        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD12 | 2        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD13 | 2        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD11 | 8        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD12 | 8        | 0.11          |
| (1,1144) | 1:157:A:LEU:HA   | 1:157:A:LEU:HD13 | 8        | 0.11          |
| (1,1027) | 1:149:A:ASP:HA   | 1:150:A:PRO:HG3  | 6        | 0.11          |
| (1,938)  | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG21 | 3        | 0.11          |
| (1,938)  | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG22 | 3        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,938) | 1:144:A:LEU:HD21 | 1:148:A:VAL:HG23 | 3        | 0.11          |
| (1,938) | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG21 | 3        | 0.11          |
| (1,938) | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG22 | 3        | 0.11          |
| (1,938) | 1:144:A:LEU:HD22 | 1:148:A:VAL:HG23 | 3        | 0.11          |
| (1,938) | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG21 | 3        | 0.11          |
| (1,938) | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG22 | 3        | 0.11          |
| (1,938) | 1:144:A:LEU:HD23 | 1:148:A:VAL:HG23 | 3        | 0.11          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 7        | 0.11          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 7        | 0.11          |
| (1,913) | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 7        | 0.11          |
| (1,882) | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG11 | 1        | 0.11          |
| (1,882) | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG12 | 1        | 0.11          |
| (1,882) | 1:142:A:TYR:HD1  | 1:165:A:VAL:HG13 | 1        | 0.11          |
| (1,882) | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG11 | 1        | 0.11          |
| (1,882) | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG12 | 1        | 0.11          |
| (1,882) | 1:142:A:TYR:HD2  | 1:165:A:VAL:HG13 | 1        | 0.11          |
| (1,842) | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 1        | 0.11          |
| (1,842) | 1:141:A:LYS:HA   | 1:141:A:LYS:HB2  | 6        | 0.11          |
| (1,779) | 1:131:A:HIS:HA   | 1:131:A:HIS:HE1  | 7        | 0.11          |
| (1,759) | 1:128:A:GLN:HG2  | 1:133:A:TYR:HA   | 1        | 0.11          |
| (1,759) | 1:128:A:GLN:HG2  | 1:133:A:TYR:HA   | 4        | 0.11          |
| (1,742) | 1:127:A:ARG:HB2  | 1:127:A:ARG:HD2  | 1        | 0.11          |
| (1,737) | 1:127:A:ARG:HA   | 1:127:A:ARG:HD3  | 10       | 0.11          |
| (1,734) | 1:127:A:ARG:HA   | 1:127:A:ARG:HB3  | 4        | 0.11          |
| (1,734) | 1:127:A:ARG:HA   | 1:127:A:ARG:HB3  | 6        | 0.11          |
| (1,734) | 1:127:A:ARG:HA   | 1:127:A:ARG:HB3  | 8        | 0.11          |
| (1,734) | 1:127:A:ARG:HA   | 1:127:A:ARG:HB3  | 10       | 0.11          |
| (1,729) | 1:126:A:GLU:HG3  | 1:133:A:TYR:HB3  | 10       | 0.11          |
| (1,719) | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD1  | 2        | 0.11          |
| (1,719) | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD2  | 2        | 0.11          |
| (1,708) | 1:126:A:GLU:HA   | 1:134:A:ILE:HG21 | 6        | 0.11          |
| (1,708) | 1:126:A:GLU:HA   | 1:134:A:ILE:HG22 | 6        | 0.11          |
| (1,708) | 1:126:A:GLU:HA   | 1:134:A:ILE:HG23 | 6        | 0.11          |
| (1,704) | 1:125:A:GLU:HA   | 1:135:A:SER:HB3  | 2        | 0.11          |
| (1,694) | 1:123:A:LYS:HD2  | 1:137:A:CYS:HA   | 9        | 0.11          |
| (1,692) | 1:123:A:LYS:HG3  | 1:137:A:CYS:HB2  | 10       | 0.11          |
| (1,671) | 1:121:A:THR:HG21 | 1:137:A:CYS:HB3  | 2        | 0.11          |
| (1,671) | 1:121:A:THR:HG22 | 1:137:A:CYS:HB3  | 2        | 0.11          |
| (1,671) | 1:121:A:THR:HG23 | 1:137:A:CYS:HB3  | 2        | 0.11          |
| (1,664) | 1:121:A:THR:HA   | 1:139:A:THR:HA   | 10       | 0.11          |
| (1,650) | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD1  | 6        | 0.11          |
| (1,650) | 1:120:A:ILE:HG21 | 1:142:A:TYR:HD2  | 6        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,650) | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD1  | 6        | 0.11          |
| (1,650) | 1:120:A:ILE:HG22 | 1:142:A:TYR:HD2  | 6        | 0.11          |
| (1,650) | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD1  | 6        | 0.11          |
| (1,650) | 1:120:A:ILE:HG23 | 1:142:A:TYR:HD2  | 6        | 0.11          |
| (1,649) | 1:120:A:ILE:HG21 | 1:140:A:ARG:HA   | 6        | 0.11          |
| (1,649) | 1:120:A:ILE:HG22 | 1:140:A:ARG:HA   | 6        | 0.11          |
| (1,649) | 1:120:A:ILE:HG23 | 1:140:A:ARG:HA   | 6        | 0.11          |
| (1,648) | 1:120:A:ILE:HG21 | 1:139:A:THR:HA   | 8        | 0.11          |
| (1,648) | 1:120:A:ILE:HG22 | 1:139:A:THR:HA   | 8        | 0.11          |
| (1,648) | 1:120:A:ILE:HG23 | 1:139:A:THR:HA   | 8        | 0.11          |
| (1,647) | 1:120:A:ILE:HG21 | 1:122:A:GLY:HA3  | 8        | 0.11          |
| (1,647) | 1:120:A:ILE:HG22 | 1:122:A:GLY:HA3  | 8        | 0.11          |
| (1,647) | 1:120:A:ILE:HG23 | 1:122:A:GLY:HA3  | 8        | 0.11          |
| (1,639) | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 6        | 0.11          |
| (1,639) | 1:120:A:ILE:HG12 | 1:121:A:THR:HA   | 7        | 0.11          |
| (1,636) | 1:120:A:ILE:HB   | 1:140:A:ARG:HD3  | 6        | 0.11          |
| (1,604) | 1:119:A:GLU:HA   | 1:120:A:ILE:HG12 | 9        | 0.11          |
| (1,571) | 1:118:A:VAL:HB   | 1:142:A:TYR:HD1  | 8        | 0.11          |
| (1,571) | 1:118:A:VAL:HB   | 1:142:A:TYR:HD2  | 8        | 0.11          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD21 | 10       | 0.11          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD22 | 10       | 0.11          |
| (1,566) | 1:118:A:VAL:HA   | 1:144:A:LEU:HD23 | 10       | 0.11          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 1        | 0.11          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 1        | 0.11          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 1        | 0.11          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG11 | 6        | 0.11          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG12 | 6        | 0.11          |
| (1,551) | 1:117:A:VAL:HA   | 1:148:A:VAL:HG13 | 6        | 0.11          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG21 | 7        | 0.11          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG22 | 7        | 0.11          |
| (1,513) | 1:115:A:ASP:HB2  | 1:117:A:VAL:HG23 | 7        | 0.11          |
| (1,502) | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 5        | 0.11          |
| (1,502) | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 5        | 0.11          |
| (1,502) | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 5        | 0.11          |
| (1,502) | 1:113:A:THR:HG21 | 1:150:A:PRO:HB3  | 10       | 0.11          |
| (1,502) | 1:113:A:THR:HG22 | 1:150:A:PRO:HB3  | 10       | 0.11          |
| (1,502) | 1:113:A:THR:HG23 | 1:150:A:PRO:HB3  | 10       | 0.11          |
| (1,484) | 1:113:A:THR:HA   | 1:118:A:VAL:HG11 | 4        | 0.11          |
| (1,484) | 1:113:A:THR:HA   | 1:118:A:VAL:HG12 | 4        | 0.11          |
| (1,484) | 1:113:A:THR:HA   | 1:118:A:VAL:HG13 | 4        | 0.11          |
| (1,395) | 1:110:A:THR:HB   | 1:112:A:LYS:HG2  | 1        | 0.11          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD21 | 8        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD22 | 8        | 0.11          |
| (1,371) | 1:109:A:LEU:HD11 | 1:157:A:LEU:HD23 | 8        | 0.11          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD21 | 8        | 0.11          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD22 | 8        | 0.11          |
| (1,371) | 1:109:A:LEU:HD12 | 1:157:A:LEU:HD23 | 8        | 0.11          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD21 | 8        | 0.11          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD22 | 8        | 0.11          |
| (1,371) | 1:109:A:LEU:HD13 | 1:157:A:LEU:HD23 | 8        | 0.11          |
| (1,332) | 1:107:A:ASP:HA   | 1:108:A:GLU:HG3  | 3        | 0.11          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD11 | 2        | 0.11          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD12 | 2        | 0.11          |
| (1,289) | 1:105:A:ALA:HA   | 1:157:A:LEU:HD13 | 2        | 0.11          |
| (1,288) | 1:105:A:ALA:HA   | 1:109:A:LEU:HD11 | 10       | 0.11          |
| (1,288) | 1:105:A:ALA:HA   | 1:109:A:LEU:HD12 | 10       | 0.11          |
| (1,288) | 1:105:A:ALA:HA   | 1:109:A:LEU:HD13 | 10       | 0.11          |
| (1,271) | 1:101:A:VAL:HG21 | 1:102:A:ASN:HA   | 8        | 0.11          |
| (1,271) | 1:101:A:VAL:HG22 | 1:102:A:ASN:HA   | 8        | 0.11          |
| (1,271) | 1:101:A:VAL:HG23 | 1:102:A:ASN:HA   | 8        | 0.11          |
| (1,261) | 1:100:A:ASP:HA   | 1:162:A:THR:HA   | 8        | 0.11          |
| (1,236) | 1:99:A:LEU:HD11  | 1:164:A:THR:HA   | 3        | 0.11          |
| (1,236) | 1:99:A:LEU:HD12  | 1:164:A:THR:HA   | 3        | 0.11          |
| (1,236) | 1:99:A:LEU:HD13  | 1:164:A:THR:HA   | 3        | 0.11          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD11 | 4        | 0.11          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD12 | 4        | 0.11          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD13 | 4        | 0.11          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD11 | 9        | 0.11          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD12 | 9        | 0.11          |
| (1,216) | 1:99:A:LEU:HB3   | 1:109:A:LEU:HD13 | 9        | 0.11          |
| (1,186) | 1:98:A:SER:HB2   | 1:164:A:THR:HA   | 10       | 0.11          |
| (1,161) | 1:97:A:VAL:HG21  | 1:166:A:GLU:HA   | 4        | 0.11          |
| (1,161) | 1:97:A:VAL:HG22  | 1:166:A:GLU:HA   | 4        | 0.11          |
| (1,161) | 1:97:A:VAL:HG23  | 1:166:A:GLU:HA   | 4        | 0.11          |
| (1,141) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD1  | 1        | 0.11          |
| (1,141) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD2  | 1        | 0.11          |
| (1,141) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD1  | 1        | 0.11          |
| (1,141) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD2  | 1        | 0.11          |
| (1,141) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD1  | 1        | 0.11          |
| (1,141) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD2  | 1        | 0.11          |
| (1,141) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD1  | 4        | 0.11          |
| (1,141) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD2  | 4        | 0.11          |
| (1,141) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD1  | 4        | 0.11          |
| (1,141) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD2  | 4        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,141)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD1  | 4        | 0.11          |
| (1,141)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD2  | 4        | 0.11          |
| (1,141)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD1  | 5        | 0.11          |
| (1,141)  | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD2  | 5        | 0.11          |
| (1,141)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD1  | 5        | 0.11          |
| (1,141)  | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD2  | 5        | 0.11          |
| (1,141)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD1  | 5        | 0.11          |
| (1,141)  | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD2  | 5        | 0.11          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG21 | 8        | 0.11          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG22 | 8        | 0.11          |
| (1,132)  | 1:97:A:VAL:HB    | 1:165:A:VAL:HG23 | 8        | 0.11          |
| (1,102)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HB3  | 4        | 0.11          |
| (1,101)  | 1:96:A:ARG:HB3   | 1:166:A:GLU:HA   | 5        | 0.11          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG21 | 3        | 0.11          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG22 | 3        | 0.11          |
| (1,100)  | 1:96:A:ARG:HB3   | 1:164:A:THR:HG23 | 3        | 0.11          |
| (1,60)   | 1:95:A:TRP:HB2   | 1:95:A:TRP:HE3   | 8        | 0.11          |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 2        | 0.11          |
| (1,45)   | 1:94:A:ARG:HG2   | 1:168:A:PRO:HB2  | 8        | 0.11          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB1   | 1        | 0.11          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB2   | 1        | 0.11          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB3   | 1        | 0.11          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB1   | 10       | 0.11          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB2   | 10       | 0.11          |
| (1,11)   | 1:91:A:THR:HB    | 1:92:A:ALA:HB3   | 10       | 0.11          |
| (1,4278) | 1:169:B:MET:H    | 1:169:B:MET:HA   | 6        | 0.1           |
| (1,4207) | 1:162:B:THR:H    | 1:161:B:GLY:HA2  | 7        | 0.1           |
| (1,4197) | 1:162:B:THR:H    | 1:102:B:ASN:HB3  | 9        | 0.1           |
| (1,4183) | 1:161:B:GLY:H    | 1:102:B:ASN:HB3  | 5        | 0.1           |
| (1,4130) | 1:155:B:SER:H    | 1:156:B:SER:HA   | 7        | 0.1           |
| (1,4037) | 1:148:B:VAL:H    | 1:170:B:PRO:HG3  | 10       | 0.1           |
| (1,4034) | 1:148:B:VAL:H    | 1:149:B:ASP:H    | 4        | 0.1           |
| (1,4034) | 1:148:B:VAL:H    | 1:149:B:ASP:H    | 8        | 0.1           |
| (1,3928) | 1:132:B:GLY:H    | 1:131:B:HIS:HB3  | 1        | 0.1           |
| (1,3928) | 1:132:B:GLY:H    | 1:131:B:HIS:HB3  | 6        | 0.1           |
| (1,3924) | 1:132:B:GLY:H    | 1:130:B:GLU:HB3  | 6        | 0.1           |
| (1,3915) | 1:131:B:HIS:H    | 1:129:B:ASP:HB3  | 5        | 0.1           |
| (1,3910) | 1:129:B:ASP:H    | 1:133:B:TYR:HB2  | 5        | 0.1           |
| (1,3905) | 1:129:B:ASP:H    | 1:131:B:HIS:HA   | 9        | 0.1           |
| (1,3894) | 1:128:B:GLN:HE21 | 1:128:B:GLN:HA   | 6        | 0.1           |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD1  | 8        | 0.1           |
| (1,3877) | 1:127:B:ARG:H    | 1:133:B:TYR:HD2  | 8        | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG21 | 1        | 0.1           |
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG22 | 1        | 0.1           |
| (1,3837) | 1:121:B:THR:H    | 1:121:B:THR:HG23 | 1        | 0.1           |
| (1,3816) | 1:120:B:ILE:H    | 1:112:B:LYS:HG3  | 10       | 0.1           |
| (1,3798) | 1:118:B:VAL:H    | 1:142:B:TYR:HB2  | 10       | 0.1           |
| (1,3770) | 1:114:B:LYS:H    | 1:119:B:GLU:H    | 5        | 0.1           |
| (1,3726) | 1:111:B:VAL:H    | 1:110:B:THR:HB   | 9        | 0.1           |
| (1,3670) | 1:105:B:ALA:H    | 1:106:B:PRO:HD3  | 2        | 0.1           |
| (1,3644) | 1:101:B:VAL:H    | 1:162:B:THR:HA   | 1        | 0.1           |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG21  | 9        | 0.1           |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG22  | 9        | 0.1           |
| (1,3600) | 1:94:B:ARG:H     | 1:91:B:THR:HG23  | 9        | 0.1           |
| (1,3585) | 1:169:B:MET:HG3  | 1:170:B:PRO:HD2  | 5        | 0.1           |
| (1,3453) | 1:157:B:LEU:HD11 | 1:163:B:LEU:HB2  | 7        | 0.1           |
| (1,3453) | 1:157:B:LEU:HD12 | 1:163:B:LEU:HB2  | 7        | 0.1           |
| (1,3453) | 1:157:B:LEU:HD13 | 1:163:B:LEU:HB2  | 7        | 0.1           |
| (1,3436) | 1:157:B:LEU:HB2  | 1:163:B:LEU:HA   | 10       | 0.1           |
| (1,3429) | 1:157:B:LEU:HA   | 1:162:B:THR:HB   | 9        | 0.1           |
| (1,3425) | 1:157:B:LEU:HA   | 1:157:B:LEU:HD11 | 7        | 0.1           |
| (1,3425) | 1:157:B:LEU:HA   | 1:157:B:LEU:HD12 | 7        | 0.1           |
| (1,3425) | 1:157:B:LEU:HA   | 1:157:B:LEU:HD13 | 7        | 0.1           |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD21 | 9        | 0.1           |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD22 | 9        | 0.1           |
| (1,3403) | 1:155:B:SER:HB3  | 1:157:B:LEU:HD23 | 9        | 0.1           |
| (1,3341) | 1:152:B:GLN:HA   | 1:168:B:PRO:HG3  | 1        | 0.1           |
| (1,3278) | 1:148:B:VAL:HB   | 1:150:B:PRO:HA   | 1        | 0.1           |
| (1,3049) | 1:129:B:ASP:HA   | 1:134:B:ILE:HG21 | 1        | 0.1           |
| (1,3049) | 1:129:B:ASP:HA   | 1:134:B:ILE:HG22 | 1        | 0.1           |
| (1,3049) | 1:129:B:ASP:HA   | 1:134:B:ILE:HG23 | 1        | 0.1           |
| (1,3043) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HD1  | 4        | 0.1           |
| (1,3043) | 1:128:B:GLN:HG3  | 1:133:B:TYR:HD2  | 4        | 0.1           |
| (1,3027) | 1:128:B:GLN:HA   | 1:128:B:GLN:HG3  | 5        | 0.1           |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD11 | 4        | 0.1           |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD12 | 4        | 0.1           |
| (1,3022) | 1:127:B:ARG:HA   | 1:134:B:ILE:HD13 | 4        | 0.1           |
| (1,3015) | 1:127:B:ARG:HA   | 1:127:B:ARG:HB3  | 10       | 0.1           |
| (1,2977) | 1:123:B:LYS:HD3  | 1:137:B:CYS:HB3  | 9        | 0.1           |
| (1,2916) | 1:120:B:ILE:HB   | 1:140:B:ARG:HD2  | 10       | 0.1           |
| (1,2900) | 1:119:B:GLU:HG2  | 1:141:B:LYS:HE3  | 7        | 0.1           |
| (1,2886) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG13 | 3        | 0.1           |
| (1,2885) | 1:119:B:GLU:HA   | 1:120:B:ILE:HG12 | 6        | 0.1           |
| (1,2831) | 1:117:B:VAL:HA   | 1:148:B:VAL:HB   | 7        | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2830) | 1:117:B:VAL:HA  | 1:144:B:LEU:HD21 | 6        | 0.1           |
| (1,2830) | 1:117:B:VAL:HA  | 1:144:B:LEU:HD22 | 6        | 0.1           |
| (1,2830) | 1:117:B:VAL:HA  | 1:144:B:LEU:HD23 | 6        | 0.1           |
| (1,2809) | 1:116:B:GLY:HA2 | 1:148:B:VAL:HB   | 10       | 0.1           |
| (1,2802) | 1:116:B:GLY:HA2 | 1:118:B:VAL:HG21 | 1        | 0.1           |
| (1,2802) | 1:116:B:GLY:HA2 | 1:118:B:VAL:HG22 | 1        | 0.1           |
| (1,2802) | 1:116:B:GLY:HA2 | 1:118:B:VAL:HG23 | 1        | 0.1           |
| (1,2704) | 1:111:B:VAL:HB  | 1:112:B:LYS:HA   | 9        | 0.1           |
| (1,2578) | 1:105:B:ALA:HB1 | 1:107:B:ASP:HB3  | 8        | 0.1           |
| (1,2578) | 1:105:B:ALA:HB2 | 1:107:B:ASP:HB3  | 8        | 0.1           |
| (1,2578) | 1:105:B:ALA:HB3 | 1:107:B:ASP:HB3  | 8        | 0.1           |
| (1,2497) | 1:99:B:LEU:HB3  | 1:109:B:LEU:HD11 | 2        | 0.1           |
| (1,2497) | 1:99:B:LEU:HB3  | 1:109:B:LEU:HD12 | 2        | 0.1           |
| (1,2497) | 1:99:B:LEU:HB3  | 1:109:B:LEU:HD13 | 2        | 0.1           |
| (1,2497) | 1:99:B:LEU:HB3  | 1:109:B:LEU:HD11 | 5        | 0.1           |
| (1,2497) | 1:99:B:LEU:HB3  | 1:109:B:LEU:HD12 | 5        | 0.1           |
| (1,2497) | 1:99:B:LEU:HB3  | 1:109:B:LEU:HD13 | 5        | 0.1           |
| (1,2430) | 1:97:B:VAL:HG21 | 1:98:B:SER:HB2   | 3        | 0.1           |
| (1,2430) | 1:97:B:VAL:HG22 | 1:98:B:SER:HB2   | 3        | 0.1           |
| (1,2430) | 1:97:B:VAL:HG23 | 1:98:B:SER:HB2   | 3        | 0.1           |
| (1,2424) | 1:97:B:VAL:HG11 | 1:142:B:TYR:HE1  | 7        | 0.1           |
| (1,2424) | 1:97:B:VAL:HG11 | 1:142:B:TYR:HE2  | 7        | 0.1           |
| (1,2424) | 1:97:B:VAL:HG12 | 1:142:B:TYR:HE1  | 7        | 0.1           |
| (1,2424) | 1:97:B:VAL:HG12 | 1:142:B:TYR:HE2  | 7        | 0.1           |
| (1,2424) | 1:97:B:VAL:HG13 | 1:142:B:TYR:HE1  | 7        | 0.1           |
| (1,2424) | 1:97:B:VAL:HG13 | 1:142:B:TYR:HE2  | 7        | 0.1           |
| (1,2422) | 1:97:B:VAL:HG11 | 1:142:B:TYR:HD1  | 2        | 0.1           |
| (1,2422) | 1:97:B:VAL:HG11 | 1:142:B:TYR:HD2  | 2        | 0.1           |
| (1,2422) | 1:97:B:VAL:HG12 | 1:142:B:TYR:HD1  | 2        | 0.1           |
| (1,2422) | 1:97:B:VAL:HG12 | 1:142:B:TYR:HD2  | 2        | 0.1           |
| (1,2422) | 1:97:B:VAL:HG13 | 1:142:B:TYR:HD1  | 2        | 0.1           |
| (1,2422) | 1:97:B:VAL:HG13 | 1:142:B:TYR:HD2  | 2        | 0.1           |
| (1,2400) | 1:97:B:VAL:HA   | 1:97:B:VAL:HG11  | 7        | 0.1           |
| (1,2400) | 1:97:B:VAL:HA   | 1:97:B:VAL:HG12  | 7        | 0.1           |
| (1,2400) | 1:97:B:VAL:HA   | 1:97:B:VAL:HG13  | 7        | 0.1           |
| (1,2389) | 1:96:B:ARG:HG3  | 1:97:B:VAL:HG21  | 9        | 0.1           |
| (1,2389) | 1:96:B:ARG:HG3  | 1:97:B:VAL:HG22  | 9        | 0.1           |
| (1,2389) | 1:96:B:ARG:HG3  | 1:97:B:VAL:HG23  | 9        | 0.1           |
| (1,2336) | 1:95:B:TRP:HA   | 1:96:B:ARG:HG3   | 8        | 0.1           |
| (1,2330) | 1:94:B:ARG:HD3  | 1:168:B:PRO:HA   | 9        | 0.1           |
| (1,2329) | 1:94:B:ARG:HD2  | 1:168:B:PRO:HA   | 9        | 0.1           |
| (1,2316) | 1:94:B:ARG:HB2  | 1:94:B:ARG:HG3   | 8        | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2304) | 1:94:B:ARG:HA    | 1:94:B:ARG:HB3   | 5        | 0.1           |
| (1,2279) | 1:143:B:THR:H    | 1:132:A:GLY:HA2  | 1        | 0.1           |
| (1,2234) | 1:135:A:SER:HB2  | 1:139:B:THR:HG21 | 4        | 0.1           |
| (1,2234) | 1:135:A:SER:HB2  | 1:139:B:THR:HG22 | 4        | 0.1           |
| (1,2234) | 1:135:A:SER:HB2  | 1:139:B:THR:HG23 | 4        | 0.1           |
| (1,2215) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 3        | 0.1           |
| (1,2146) | 1:143:B:THR:H    | 1:132:A:GLY:HA2  | 1        | 0.1           |
| (1,2102) | 1:135:A:SER:HB2  | 1:139:B:THR:HG21 | 4        | 0.1           |
| (1,2102) | 1:135:A:SER:HB2  | 1:139:B:THR:HG22 | 4        | 0.1           |
| (1,2102) | 1:135:A:SER:HB2  | 1:139:B:THR:HG23 | 4        | 0.1           |
| (1,2083) | 1:134:A:ILE:HG12 | 1:140:B:ARG:HB3  | 3        | 0.1           |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD11 | 7        | 0.1           |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD12 | 7        | 0.1           |
| (1,1938) | 1:164:A:THR:H    | 1:157:A:LEU:HD13 | 7        | 0.1           |
| (1,1834) | 1:154:A:SER:H    | 1:155:A:SER:HB2  | 8        | 0.1           |
| (1,1806) | 1:152:A:GLN:HE22 | 1:149:A:ASP:HB2  | 1        | 0.1           |
| (1,1804) | 1:152:A:GLN:HE21 | 1:169:A:MET:HA   | 3        | 0.1           |
| (1,1783) | 1:152:A:GLN:H    | 1:149:A:ASP:HA   | 6        | 0.1           |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD11 | 9        | 0.1           |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD12 | 9        | 0.1           |
| (1,1726) | 1:144:A:LEU:H    | 1:144:A:LEU:HD13 | 9        | 0.1           |
| (1,1668) | 1:135:A:SER:H    | 1:135:A:SER:HB3  | 2        | 0.1           |
| (1,1637) | 1:131:A:HIS:H    | 1:130:A:GLU:HG3  | 2        | 0.1           |
| (1,1616) | 1:128:A:GLN:HE21 | 1:128:A:GLN:HG2  | 7        | 0.1           |
| (1,1585) | 1:126:A:GLU:H    | 1:125:A:GLU:HA   | 7        | 0.1           |
| (1,1580) | 1:125:A:GLU:H    | 1:108:A:GLU:HG2  | 6        | 0.1           |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD21 | 8        | 0.1           |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD22 | 8        | 0.1           |
| (1,1569) | 1:123:A:LYS:H    | 1:109:A:LEU:HD23 | 8        | 0.1           |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD11 | 1        | 0.1           |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD12 | 1        | 0.1           |
| (1,1568) | 1:123:A:LYS:H    | 1:109:A:LEU:HD13 | 1        | 0.1           |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB1  | 2        | 0.1           |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB2  | 2        | 0.1           |
| (1,1563) | 1:123:A:LYS:H    | 1:105:A:ALA:HB3  | 2        | 0.1           |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG21 | 7        | 0.1           |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG22 | 7        | 0.1           |
| (1,1554) | 1:121:A:THR:H    | 1:120:A:ILE:HG23 | 7        | 0.1           |
| (1,1553) | 1:121:A:THR:H    | 1:120:A:ILE:HG13 | 10       | 0.1           |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD11 | 8        | 0.1           |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD12 | 8        | 0.1           |
| (1,1540) | 1:120:A:ILE:H    | 1:120:A:ILE:HD13 | 8        | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1517) | 1:118:A:VAL:H    | 1:142:A:TYR:HB2  | 2        | 0.1           |
| (1,1505) | 1:117:A:VAL:H    | 1:117:A:VAL:HG21 | 9        | 0.1           |
| (1,1505) | 1:117:A:VAL:H    | 1:117:A:VAL:HG22 | 9        | 0.1           |
| (1,1505) | 1:117:A:VAL:H    | 1:117:A:VAL:HG23 | 9        | 0.1           |
| (1,1458) | 1:112:A:LYS:H    | 1:112:A:LYS:HB3  | 9        | 0.1           |
| (1,1442) | 1:110:A:THR:H    | 1:122:A:GLY:H    | 8        | 0.1           |
| (1,1311) | 1:170:A:PRO:HB2  | 1:170:A:PRO:HG2  | 4        | 0.1           |
| (1,1217) | 1:161:A:GLY:HA3  | 1:163:A:LEU:HA   | 6        | 0.1           |
| (1,1198) | 1:159:A:PRO:HA   | 1:159:A:PRO:HB3  | 2        | 0.1           |
| (1,1157) | 1:157:A:LEU:HB3  | 1:157:A:LEU:HG   | 6        | 0.1           |
| (1,1079) | 1:153:A:VAL:HB   | 1:154:A:SER:HA   | 9        | 0.1           |
| (1,997)  | 1:148:A:VAL:HB   | 1:150:A:PRO:HA   | 3        | 0.1           |
| (1,992)  | 1:148:A:VAL:HA   | 1:170:A:PRO:HB3  | 2        | 0.1           |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG21 | 8        | 0.1           |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG22 | 8        | 0.1           |
| (1,913)  | 1:144:A:LEU:HB2  | 1:148:A:VAL:HG23 | 8        | 0.1           |
| (1,857)  | 1:141:A:LYS:HG2  | 1:143:A:THR:HA   | 5        | 0.1           |
| (1,853)  | 1:141:A:LYS:HG2  | 1:141:A:LYS:HE3  | 3        | 0.1           |
| (1,782)  | 1:131:A:HIS:HB2  | 1:132:A:GLY:HA2  | 7        | 0.1           |
| (1,776)  | 1:130:A:GLU:HG3  | 1:131:A:HIS:HD2  | 6        | 0.1           |
| (1,719)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD1  | 7        | 0.1           |
| (1,719)  | 1:126:A:GLU:HG2  | 1:133:A:TYR:HD2  | 7        | 0.1           |
| (1,712)  | 1:126:A:GLU:HB3  | 1:133:A:TYR:HB2  | 4        | 0.1           |
| (1,654)  | 1:120:A:ILE:HD11 | 1:140:A:ARG:HD2  | 8        | 0.1           |
| (1,654)  | 1:120:A:ILE:HD12 | 1:140:A:ARG:HD2  | 8        | 0.1           |
| (1,654)  | 1:120:A:ILE:HD13 | 1:140:A:ARG:HD2  | 8        | 0.1           |
| (1,649)  | 1:120:A:ILE:HG21 | 1:140:A:ARG:HA   | 9        | 0.1           |
| (1,649)  | 1:120:A:ILE:HG22 | 1:140:A:ARG:HA   | 9        | 0.1           |
| (1,649)  | 1:120:A:ILE:HG23 | 1:140:A:ARG:HA   | 9        | 0.1           |
| (1,613)  | 1:119:A:GLU:HB3  | 1:121:A:THR:HB   | 6        | 0.1           |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD1  | 5        | 0.1           |
| (1,585)  | 1:118:A:VAL:HG11 | 1:142:A:TYR:HD2  | 5        | 0.1           |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD1  | 5        | 0.1           |
| (1,585)  | 1:118:A:VAL:HG12 | 1:142:A:TYR:HD2  | 5        | 0.1           |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD1  | 5        | 0.1           |
| (1,585)  | 1:118:A:VAL:HG13 | 1:142:A:TYR:HD2  | 5        | 0.1           |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD21 | 7        | 0.1           |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD22 | 7        | 0.1           |
| (1,566)  | 1:118:A:VAL:HA   | 1:144:A:LEU:HD23 | 7        | 0.1           |
| (1,562)  | 1:117:A:VAL:HG11 | 1:142:A:TYR:HB3  | 2        | 0.1           |
| (1,562)  | 1:117:A:VAL:HG12 | 1:142:A:TYR:HB3  | 2        | 0.1           |
| (1,562)  | 1:117:A:VAL:HG13 | 1:142:A:TYR:HB3  | 2        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,553) | 1:117:A:VAL:HB   | 1:143:A:THR:HA   | 10       | 0.1           |
| (1,517) | 1:115:A:ASP:HB3  | 1:150:A:PRO:HG2  | 6        | 0.1           |
| (1,466) | 1:112:A:LYS:HG3  | 1:119:A:GLU:HA   | 3        | 0.1           |
| (1,453) | 1:112:A:LYS:HA   | 1:114:A:LYS:HB3  | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG21 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG22 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG11 | 1:118:A:VAL:HG23 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG21 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG22 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG12 | 1:118:A:VAL:HG23 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG21 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG22 | 5        | 0.1           |
| (1,432) | 1:111:A:VAL:HG13 | 1:118:A:VAL:HG23 | 5        | 0.1           |
| (1,288) | 1:105:A:ALA:HA   | 1:109:A:LEU:HD11 | 3        | 0.1           |
| (1,288) | 1:105:A:ALA:HA   | 1:109:A:LEU:HD12 | 3        | 0.1           |
| (1,288) | 1:105:A:ALA:HA   | 1:109:A:LEU:HD13 | 3        | 0.1           |
| (1,248) | 1:99:A:LEU:HD21  | 1:140:A:ARG:HD2  | 1        | 0.1           |
| (1,248) | 1:99:A:LEU:HD22  | 1:140:A:ARG:HD2  | 1        | 0.1           |
| (1,248) | 1:99:A:LEU:HD23  | 1:140:A:ARG:HD2  | 1        | 0.1           |
| (1,143) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE1  | 2        | 0.1           |
| (1,143) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE2  | 2        | 0.1           |
| (1,143) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE1  | 2        | 0.1           |
| (1,143) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE2  | 2        | 0.1           |
| (1,143) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE1  | 2        | 0.1           |
| (1,143) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE2  | 2        | 0.1           |
| (1,143) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE1  | 9        | 0.1           |
| (1,143) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HE2  | 9        | 0.1           |
| (1,143) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE1  | 9        | 0.1           |
| (1,143) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HE2  | 9        | 0.1           |
| (1,143) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE1  | 9        | 0.1           |
| (1,143) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HE2  | 9        | 0.1           |
| (1,141) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD1  | 9        | 0.1           |
| (1,141) | 1:97:A:VAL:HG11  | 1:142:A:TYR:HD2  | 9        | 0.1           |
| (1,141) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD1  | 9        | 0.1           |
| (1,141) | 1:97:A:VAL:HG12  | 1:142:A:TYR:HD2  | 9        | 0.1           |
| (1,141) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD1  | 9        | 0.1           |
| (1,141) | 1:97:A:VAL:HG13  | 1:142:A:TYR:HD2  | 9        | 0.1           |
| (1,132) | 1:97:A:VAL:HB    | 1:165:A:VAL:HG21 | 7        | 0.1           |
| (1,132) | 1:97:A:VAL:HB    | 1:165:A:VAL:HG22 | 7        | 0.1           |
| (1,132) | 1:97:A:VAL:HB    | 1:165:A:VAL:HG23 | 7        | 0.1           |
| (1,116) | 1:96:A:ARG:HD3   | 1:166:A:GLU:HB3  | 9        | 0.1           |

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

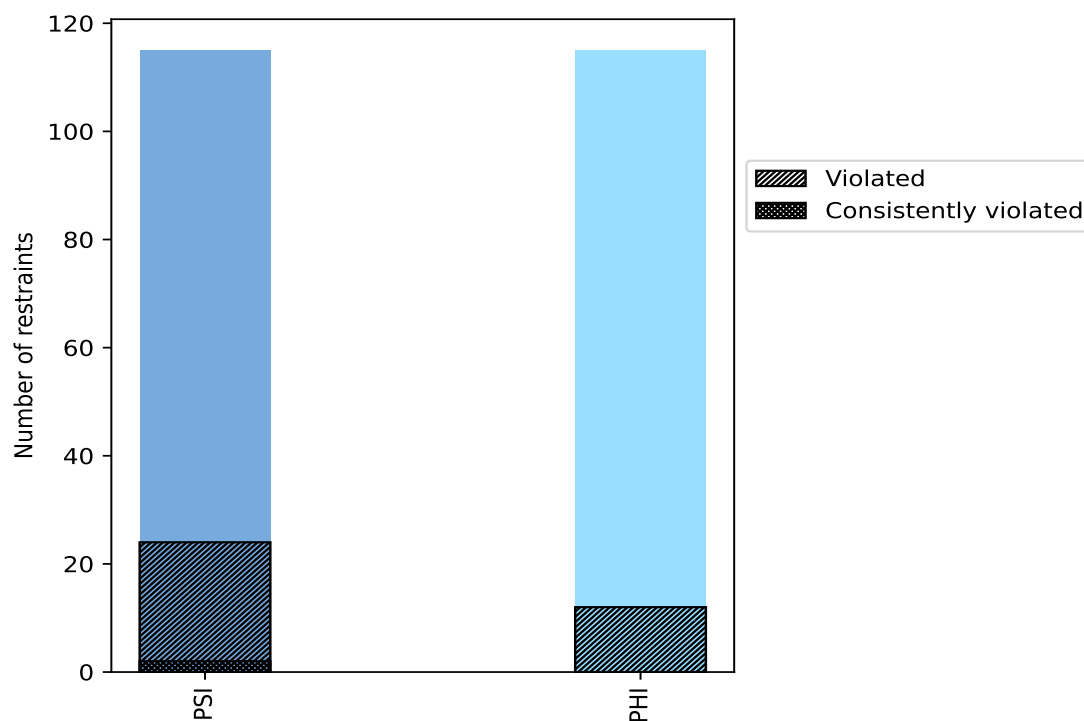
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 115   | 50.0           | 24                    | 20.9           | 10.4           | 2                                  | 1.7            | 0.9            |
| PHI        | 115   | 50.0           | 12                    | 10.4           | 5.2            | 0                                  | 0.0            | 0.0            |
| Total      | 230   | 100.0          | 36                    | 15.7           | 15.7           | 2                                  | 0.9            | 0.9            |

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

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



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

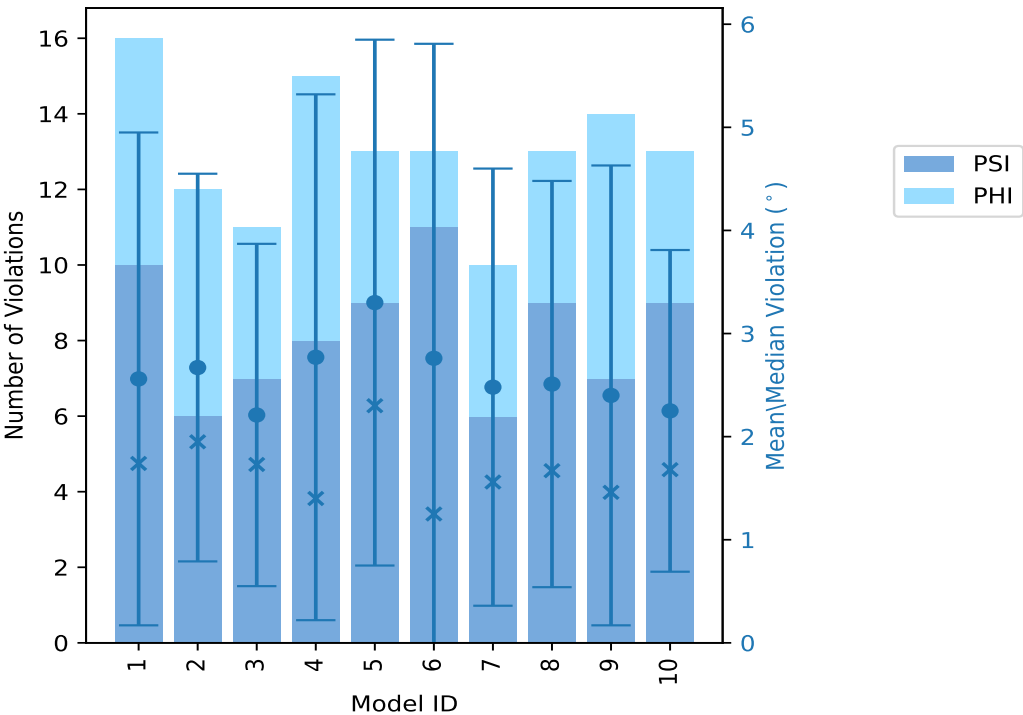


10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 10                   | 6   | 16    | 2.56     | 9.21    | 2.39   | 1.74       |
| 2        | 6                    | 6   | 12    | 2.67     | 7.82    | 1.88   | 1.95       |
| 3        | 7                    | 4   | 11    | 2.21     | 7.02    | 1.66   | 1.73       |
| 4        | 8                    | 7   | 15    | 2.77     | 9.05    | 2.55   | 1.4        |
| 5        | 9                    | 4   | 13    | 3.3      | 9.77    | 2.55   | 2.3        |
| 6        | 11                   | 2   | 13    | 2.76     | 10.01   | 3.05   | 1.25       |
| 7        | 6                    | 4   | 10    | 2.48     | 7.7     | 2.12   | 1.56       |
| 8        | 9                    | 4   | 13    | 2.51     | 7.46    | 1.97   | 1.67       |
| 9        | 7                    | 7   | 14    | 2.4      | 8.65    | 2.23   | 1.46       |
| 10       | 9                    | 4   | 13    | 2.25     | 7.26    | 1.56   | 1.68       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

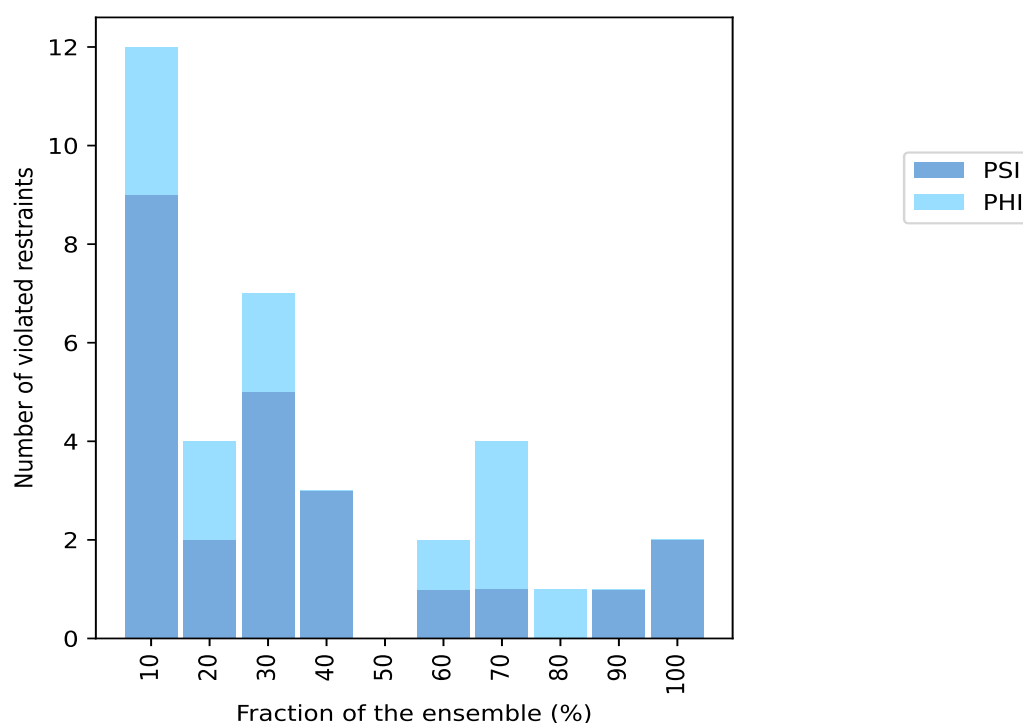
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 9                             | 3   | 12    | 1                        | 10.0  |
| 2                             | 2   | 4     | 2                        | 20.0  |
| 5                             | 2   | 7     | 3                        | 30.0  |
| 3                             | 0   | 3     | 4                        | 40.0  |
| 0                             | 0   | 0     | 5                        | 50.0  |
| 1                             | 1   | 2     | 6                        | 60.0  |
| 1                             | 3   | 4     | 7                        | 70.0  |
| 0                             | 1   | 1     | 8                        | 80.0  |
| 1                             | 0   | 1     | 9                        | 90.0  |
| 2                             | 0   | 2     | 10                       | 100.0 |

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

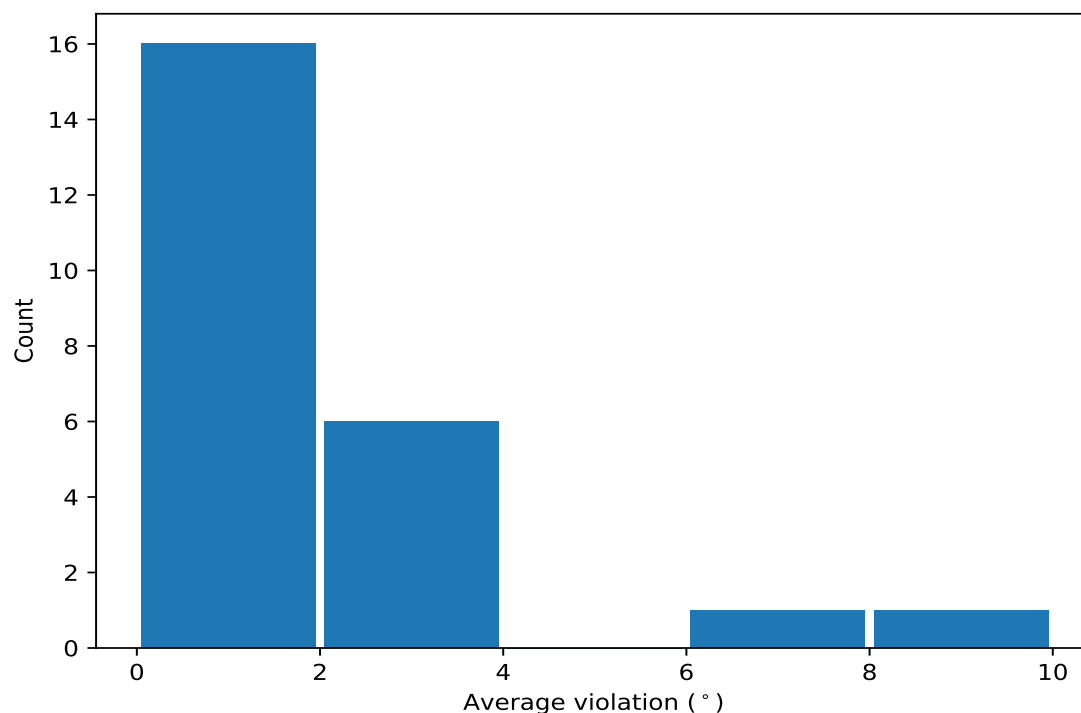
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 10                  | 8.08 | 0.98            | 7.94   |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 10                  | 6.86 | 2.25            | 7.08   |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 9                   | 1.72 | 0.53            | 1.73   |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 8                   | 2.18 | 0.49            | 2.26   |
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 7                   | 2.5  | 1.21            | 1.91   |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 7                   | 1.64 | 0.43            | 1.61   |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 7                   | 1.58 | 0.3             | 1.66   |
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 7                   | 1.46 | 0.12            | 1.51   |
| (1,30)  | 1:116:A:GLY:C | 1:117:A:VAL:N  | 1:117:A:VAL:CA | 1:117:A:VAL:C | 6                   | 1.83 | 0.4             | 1.89   |
| (1,132) | 1:107:B:ASP:N | 1:107:B:ASP:CA | 1:107:B:ASP:C  | 1:108:B:GLU:N | 6                   | 1.46 | 0.35            | 1.34   |
| (1,163) | 1:126:B:GLU:N | 1:126:B:GLU:CA | 1:126:B:GLU:C  | 1:127:B:ARG:N | 4                   | 2.15 | 0.59            | 1.96   |
| (1,144) | 1:115:B:ASP:N | 1:115:B:ASP:CA | 1:115:B:ASP:C  | 1:116:B:GLY:N | 4                   | 2.0  | 0.74            | 1.85   |
| (1,28)  | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:GLY:N | 4                   | 1.53 | 0.22            | 1.54   |

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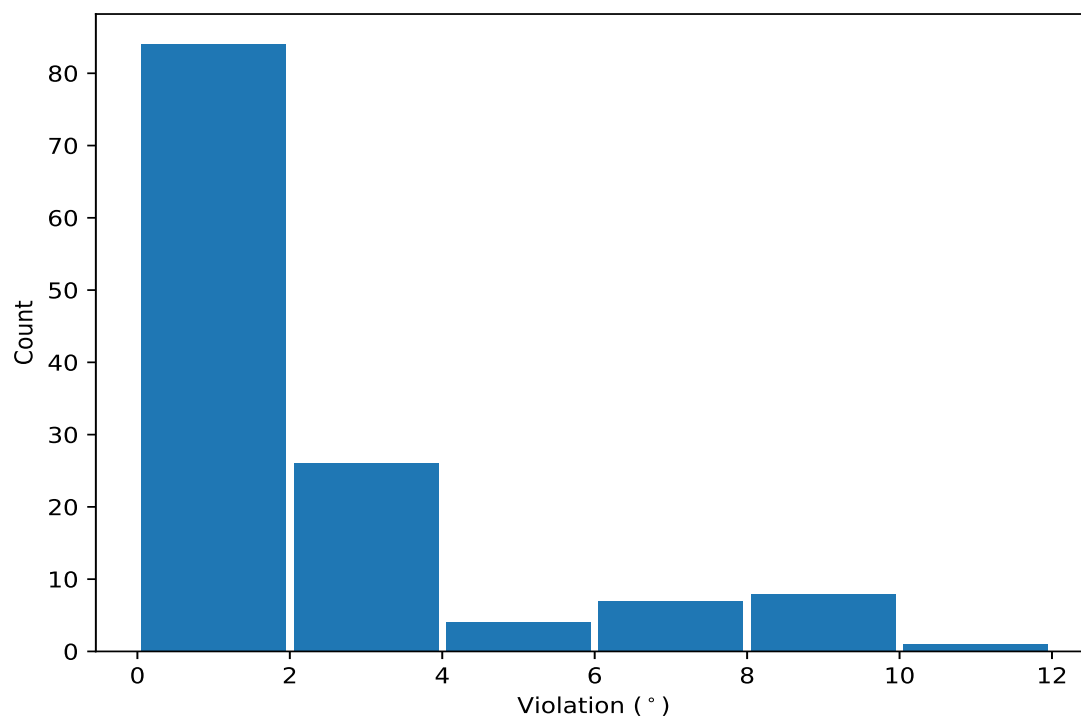
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,57)  | 1:131:A:HIS:N | 1:131:A:HIS:CA | 1:131:A:HIS:C  | 1:132:A:GLY:N | 3                   | 2.2  | 1.0             | 1.81   |
| (1,115) | 1:168:A:PRO:N | 1:168:A:PRO:CA | 1:168:A:PRO:C  | 1:169:A:MET:N | 3                   | 2.06 | 1.14            | 1.27   |
| (1,47)  | 1:126:A:GLU:N | 1:126:A:GLU:CA | 1:126:A:GLU:C  | 1:127:A:ARG:N | 3                   | 1.55 | 0.52            | 1.21   |
| (1,105) | 1:161:A:GLY:N | 1:161:A:GLY:CA | 1:161:A:GLY:C  | 1:162:A:THR:N | 3                   | 1.39 | 0.28            | 1.47   |
| (1,203) | 1:150:B:PRO:C | 1:151:B:THR:N  | 1:151:B:THR:CA | 1:151:B:THR:C | 3                   | 1.36 | 0.17            | 1.36   |
| (1,221) | 1:161:B:GLY:N | 1:161:B:GLY:CA | 1:161:B:GLY:C  | 1:162:B:THR:N | 3                   | 1.27 | 0.21            | 1.16   |
| (1,201) | 1:149:B:ASP:C | 1:150:B:PRO:N  | 1:150:B:PRO:CA | 1:150:B:PRO:C | 3                   | 1.19 | 0.15            | 1.12   |
| (1,174) | 1:132:B:GLY:C | 1:133:B:TYR:N  | 1:133:B:TYR:CA | 1:133:B:TYR:C | 2                   | 1.77 | 0.2             | 1.77   |
| (1,112) | 1:165:A:VAL:N | 1:165:A:VAL:CA | 1:165:A:VAL:C  | 1:166:A:GLU:N | 2                   | 1.34 | 0.31            | 1.34   |
| (1,42)  | 1:122:A:GLY:C | 1:123:A:LYS:N  | 1:123:A:LYS:CA | 1:123:A:LYS:C | 2                   | 1.23 | 0.1             | 1.23   |
| (1,79)  | 1:143:A:THR:N | 1:143:A:THR:CA | 1:143:A:THR:C  | 1:144:A:LEU:N | 2                   | 1.08 | 0.01            | 1.08   |

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

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

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

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



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

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

restraint.

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 6        | 10.01         |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 5        | 9.77          |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 6        | 9.52          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 1        | 9.21          |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 4        | 9.05          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 9        | 8.65          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 4        | 8.48          |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 1        | 8.31          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 5        | 8.06          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 2        | 7.82          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 7        | 7.7           |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 8        | 7.46          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 10       | 7.26          |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 3        | 7.02          |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 9        | 6.7           |
| (1,81)  | 1:144:A:LEU:N | 1:144:A:LEU:CA | 1:144:A:LEU:C  | 1:145:A:PRO:N | 8        | 6.6           |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 2        | 5.54          |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 7        | 5.46          |
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 5        | 4.46          |
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 4        | 4.31          |
| (1,115) | 1:168:A:PRO:N | 1:168:A:PRO:CA | 1:168:A:PRO:C  | 1:169:A:MET:N | 4        | 3.67          |
| (1,57)  | 1:131:A:HIS:N | 1:131:A:HIS:CA | 1:131:A:HIS:C  | 1:132:A:GLY:N | 6        | 3.57          |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 3        | 3.51          |
| (1,197) | 1:144:B:LEU:N | 1:144:B:LEU:CA | 1:144:B:LEU:C  | 1:145:B:PRO:N | 10       | 3.28          |
| (1,144) | 1:115:B:ASP:N | 1:115:B:ASP:CA | 1:115:B:ASP:C  | 1:116:B:GLY:N | 5        | 3.09          |
| (1,163) | 1:126:B:GLU:N | 1:126:B:GLU:CA | 1:126:B:GLU:C  | 1:127:B:ARG:N | 1        | 3.06          |
| (1,158) | 1:122:B:GLY:C | 1:123:B:LYS:N  | 1:123:B:LYS:CA | 1:123:B:LYS:C | 4        | 2.82          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 10       | 2.69          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 5        | 2.66          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 8        | 2.54          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 2        | 2.46          |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 9        | 2.46          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 5        | 2.42          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 9        | 2.35          |
| (1,163) | 1:126:B:GLU:N | 1:126:B:GLU:CA | 1:126:B:GLU:C  | 1:127:B:ARG:N | 5        | 2.3           |
| (1,47)  | 1:126:A:GLU:N | 1:126:A:GLU:CA | 1:126:A:GLU:C  | 1:127:A:ARG:N | 10       | 2.29          |
| (1,30)  | 1:116:A:GLY:C | 1:117:A:VAL:N  | 1:117:A:VAL:CA | 1:117:A:VAL:C | 5        | 2.27          |
| (1,144) | 1:115:B:ASP:N | 1:115:B:ASP:CA | 1:115:B:ASP:C  | 1:116:B:GLY:N | 2        | 2.23          |
| (1,132) | 1:107:B:ASP:N | 1:107:B:ASP:CA | 1:107:B:ASP:C  | 1:108:B:GLU:N | 5        | 2.21          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 2        | 2.17          |
| (1,59)  | 1:133:A:TYR:N | 1:133:A:TYR:CA | 1:133:A:TYR:C  | 1:134:A:ILE:N | 4        | 2.15          |
| (1,30)  | 1:116:A:GLY:C | 1:117:A:VAL:N  | 1:117:A:VAL:CA | 1:117:A:VAL:C | 8        | 2.14          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 8        | 2.12          |
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 3        | 2.09          |
| (1,44)  | 1:123:A:LYS:C | 1:124:A:HIS:N  | 1:124:A:HIS:CA | 1:124:A:HIS:C | 1        | 2.05          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 1        | 2.02          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1        | 1.99          |
| (1,174) | 1:132:B:GLY:C | 1:133:B:TYR:N  | 1:133:B:TYR:CA | 1:133:B:TYR:C | 9        | 1.97          |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 2        | 1.97          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 3        | 1.96          |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 2        | 1.93          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 7        | 1.91          |
| (1,30)  | 1:116:A:GLY:C | 1:117:A:VAL:N  | 1:117:A:VAL:CA | 1:117:A:VAL:C | 2        | 1.9           |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 1        | 1.9           |
| (1,30)  | 1:116:A:GLY:C | 1:117:A:VAL:N  | 1:117:A:VAL:CA | 1:117:A:VAL:C | 10       | 1.88          |
| (1,28)  | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:GLY:N | 9        | 1.83          |
| (1,57)  | 1:131:A:HIS:N | 1:131:A:HIS:CA | 1:131:A:HIS:C  | 1:132:A:GLY:N | 10       | 1.81          |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 8        | 1.79          |
| (1,45)  | 1:124:A:HIS:N | 1:124:A:HIS:CA | 1:124:A:HIS:C  | 1:125:A:GLU:N | 1        | 1.78          |
| (1,30)  | 1:116:A:GLY:C | 1:117:A:VAL:N  | 1:117:A:VAL:CA | 1:117:A:VAL:C | 3        | 1.77          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 3        | 1.73          |
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 1        | 1.69          |
| (1,105) | 1:161:A:GLY:N | 1:161:A:GLY:CA | 1:161:A:GLY:C  | 1:162:A:THR:N | 10       | 1.68          |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 8        | 1.67          |
| (1,112) | 1:165:A:VAL:N | 1:165:A:VAL:CA | 1:165:A:VAL:C  | 1:166:A:GLU:N | 6        | 1.66          |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 10       | 1.66          |
| (1,163) | 1:126:B:GLU:N | 1:126:B:GLU:CA | 1:126:B:GLU:C  | 1:127:B:ARG:N | 6        | 1.63          |
| (1,169) | 1:129:B:ASP:N | 1:129:B:ASP:CA | 1:129:B:ASP:C  | 1:130:B:GLU:N | 8        | 1.62          |
| (1,163) | 1:126:B:GLU:N | 1:126:B:GLU:CA | 1:126:B:GLU:C  | 1:127:B:ARG:N | 8        | 1.61          |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 7        | 1.61          |
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 2        | 1.59          |
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 10       | 1.58          |
| (1,203) | 1:150:B:PRO:C | 1:151:B:THR:N  | 1:151:B:THR:CA | 1:151:B:THR:C | 2        | 1.57          |
| (1,174) | 1:132:B:GLY:C | 1:133:B:TYR:N  | 1:133:B:TYR:CA | 1:133:B:TYR:C | 7        | 1.57          |
| (1,221) | 1:161:B:GLY:N | 1:161:B:GLY:CA | 1:161:B:GLY:C  | 1:162:B:THR:N | 7        | 1.56          |
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 7        | 1.56          |
| (1,28)  | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:GLY:N | 8        | 1.55          |
| (1,172) | 1:130:B:GLU:C | 1:131:B:HIS:N  | 1:131:B:HIS:CA | 1:131:B:HIS:C | 1        | 1.54          |
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 4        | 1.53          |
| (1,28)  | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:GLY:N | 2        | 1.53          |
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 3        | 1.51          |
| (1,144) | 1:115:B:ASP:N | 1:115:B:ASP:CA | 1:115:B:ASP:C  | 1:116:B:GLY:N | 6        | 1.47          |
| (1,105) | 1:161:A:GLY:N | 1:161:A:GLY:CA | 1:161:A:GLY:C  | 1:162:A:THR:N | 5        | 1.47          |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 5        | 1.47          |
| (1,132) | 1:107:B:ASP:N | 1:107:B:ASP:CA | 1:107:B:ASP:C  | 1:108:B:GLU:N | 9        | 1.46          |
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 9        | 1.45          |
| (1,104) | 1:160:A:GLU:N | 1:160:A:GLU:CA | 1:160:A:GLU:C  | 1:161:A:GLY:N | 3        | 1.45          |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 5        | 1.45          |
| (1,58)  | 1:132:A:GLY:C | 1:133:A:TYR:N  | 1:133:A:TYR:CA | 1:133:A:TYR:C | 10       | 1.45          |
| (1,132) | 1:107:B:ASP:N | 1:107:B:ASP:CA | 1:107:B:ASP:C  | 1:108:B:GLU:N | 1        | 1.43          |
| (1,201) | 1:149:B:ASP:C | 1:150:B:PRO:N  | 1:150:B:PRO:CA | 1:150:B:PRO:C | 4        | 1.4           |
| (1,203) | 1:150:B:PRO:C | 1:151:B:THR:N  | 1:151:B:THR:CA | 1:151:B:THR:C | 9        | 1.36          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 10       | 1.36          |
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 1        | 1.35          |
| (1,42)  | 1:122:A:GLY:C | 1:123:A:LYS:N  | 1:123:A:LYS:CA | 1:123:A:LYS:C | 2        | 1.32          |
| (1,115) | 1:168:A:PRO:N | 1:168:A:PRO:CA | 1:168:A:PRO:C  | 1:169:A:MET:N | 5        | 1.27          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 4        | 1.26          |
| (1,117) | 1:96:B:ARG:N  | 1:96:B:ARG:CA  | 1:96:B:ARG:C   | 1:97:B:VAL:N  | 1        | 1.26          |
| (1,132) | 1:107:B:ASP:N | 1:107:B:ASP:CA | 1:107:B:ASP:C  | 1:108:B:GLU:N | 6        | 1.25          |
| (1,115) | 1:168:A:PRO:N | 1:168:A:PRO:CA | 1:168:A:PRO:C  | 1:169:A:MET:N | 10       | 1.25          |
| (1,57)  | 1:131:A:HIS:N | 1:131:A:HIS:CA | 1:131:A:HIS:C  | 1:132:A:GLY:N | 9        | 1.22          |
| (1,28)  | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:GLY:N | 1        | 1.22          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,146) | 1:116:B:GLY:C | 1:117:B:VAL:N  | 1:117:B:VAL:CA | 1:117:B:VAL:C | 8        | 1.21          |
| (1,47)  | 1:126:A:GLU:N | 1:126:A:GLU:CA | 1:126:A:GLU:C  | 1:127:A:ARG:N | 6        | 1.21          |
| (1,132) | 1:107:B:ASP:N | 1:107:B:ASP:CA | 1:107:B:ASP:C  | 1:108:B:GLU:N | 4        | 1.2           |
| (1,132) | 1:107:B:ASP:N | 1:107:B:ASP:CA | 1:107:B:ASP:C  | 1:108:B:GLU:N | 8        | 1.2           |
| (1,144) | 1:115:B:ASP:N | 1:115:B:ASP:CA | 1:115:B:ASP:C  | 1:116:B:GLY:N | 3        | 1.19          |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 4        | 1.19          |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 7        | 1.18          |
| (1,10)  | 1:102:A:ASN:N | 1:102:A:ASN:CA | 1:102:A:ASN:C  | 1:103:A:HIS:N | 7        | 1.18          |
| (1,221) | 1:161:B:GLY:N | 1:161:B:GLY:CA | 1:161:B:GLY:C  | 1:162:B:THR:N | 6        | 1.16          |
| (1,203) | 1:150:B:PRO:C | 1:151:B:THR:N  | 1:151:B:THR:CA | 1:151:B:THR:C | 4        | 1.15          |
| (1,47)  | 1:126:A:GLU:N | 1:126:A:GLU:CA | 1:126:A:GLU:C  | 1:127:A:ARG:N | 8        | 1.15          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 6        | 1.14          |
| (1,87)  | 1:150:A:PRO:C | 1:151:A:THR:N  | 1:151:A:THR:CA | 1:151:A:THR:C | 1        | 1.14          |
| (1,42)  | 1:122:A:GLY:C | 1:123:A:LYS:N  | 1:123:A:LYS:CA | 1:123:A:LYS:C | 9        | 1.13          |
| (1,16)  | 1:107:A:ASP:N | 1:107:A:ASP:CA | 1:107:A:ASP:C  | 1:108:A:GLU:N | 4        | 1.13          |
| (1,1)   | 1:96:A:ARG:N  | 1:96:A:ARG:CA  | 1:96:A:ARG:C   | 1:97:A:VAL:N  | 6        | 1.13          |
| (1,201) | 1:149:B:ASP:C | 1:150:B:PRO:N  | 1:150:B:PRO:CA | 1:150:B:PRO:C | 6        | 1.12          |
| (1,85)  | 1:149:A:ASP:C | 1:150:A:PRO:N  | 1:150:A:PRO:CA | 1:150:A:PRO:C | 4        | 1.1           |
| (1,221) | 1:161:B:GLY:N | 1:161:B:GLY:CA | 1:161:B:GLY:C  | 1:162:B:THR:N | 4        | 1.09          |
| (1,173) | 1:131:B:HIS:N | 1:131:B:HIS:CA | 1:131:B:HIS:C  | 1:132:B:GLY:N | 7        | 1.08          |
| (1,79)  | 1:143:A:THR:N | 1:143:A:THR:CA | 1:143:A:THR:C  | 1:144:A:LEU:N | 10       | 1.08          |
| (1,79)  | 1:143:A:THR:N | 1:143:A:THR:CA | 1:143:A:THR:C  | 1:144:A:LEU:N | 1        | 1.07          |
| (1,228) | 1:165:B:VAL:N | 1:165:B:VAL:CA | 1:165:B:VAL:C  | 1:166:B:GLU:N | 3        | 1.06          |
| (1,201) | 1:149:B:ASP:C | 1:150:B:PRO:N  | 1:150:B:PRO:CA | 1:150:B:PRO:C | 9        | 1.05          |
| (1,112) | 1:165:A:VAL:N | 1:165:A:VAL:CA | 1:165:A:VAL:C  | 1:166:A:GLU:N | 3        | 1.03          |
| (1,30)  | 1:116:A:GLY:C | 1:117:A:VAL:N  | 1:117:A:VAL:CA | 1:117:A:VAL:C | 6        | 1.03          |
| (1,105) | 1:161:A:GLY:N | 1:161:A:GLY:CA | 1:161:A:GLY:C  | 1:162:A:THR:N | 9        | 1.02          |
| (1,193) | 1:142:B:TYR:N | 1:142:B:TYR:CA | 1:142:B:TYR:C  | 1:143:B:THR:N | 9        | 1.0           |