



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 12:34 AM EST

PDB ID : 2N2H  
BMRB ID : 25599  
Title : Solution structure of Sds3 in complex with Sin3A  
Authors : Clark, M.; Radhakrishnan, I.  
Deposited on : 2015-05-08

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 : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

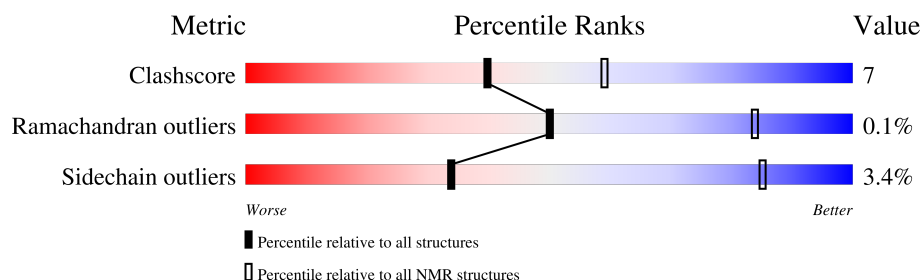
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 83%.

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            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

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     | 27     |                  |
| 2   | B     | 125    |                  |

## 2 Ensemble composition and analysis

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

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

| Well-defined (core) protein residues |  |                   |              |
|--------------------------------------|--|-------------------|--------------|
| Well-defined core                    | Residue range (total)                          | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:207-A:224, B:616-B:658,<br>B:662-B:716 (116) | 0.74              | 1            |

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

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

The models can be grouped into 5 clusters and 6 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2537 atoms, of which 1285 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sin3 histone deacetylase corepressor complex component SDS3.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 27       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 442   | 134 | 224 | 37 | 46 | 1 |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 202     | SER      | -      | expression tag | UNP Q8BR65 |
| A     | 203     | ASN      | -      | expression tag | UNP Q8BR65 |
| A     | 204     | ALA      | -      | expression tag | UNP Q8BR65 |

- Molecule 2 is a protein called Paired amphipathic helix protein Sin3a.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 2   | B     | 125      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2095  | 649 | 1061 | 190 | 193 | 2 |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 605     | SER      | -      | expression tag | UNP Q60520 |
| B     | 606     | ASN      | -      | expression tag | UNP Q60520 |
| B     | 607     | ALA      | -      | expression tag | UNP Q60520 |

## 4 Residue-property plots

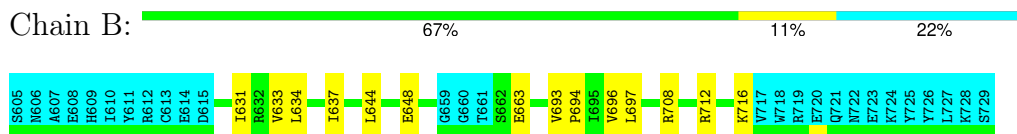
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



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

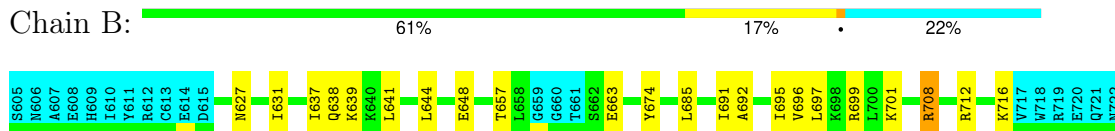
Colouring as in section 4.1 above.

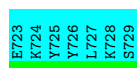
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



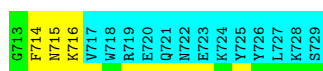


#### 4.2.2 Score per residue for model 2

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a

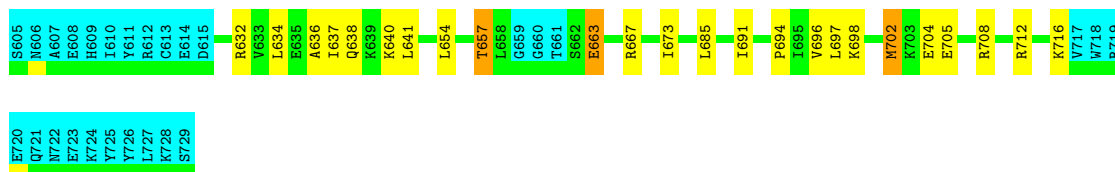


#### 4.2.3 Score per residue for model 3

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



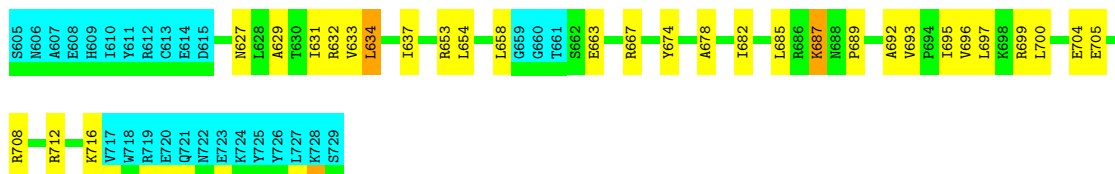
#### 4.2.4 Score per residue for model 4

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3





- Molecule 2: Paired amphipathic helix protein Sin3a

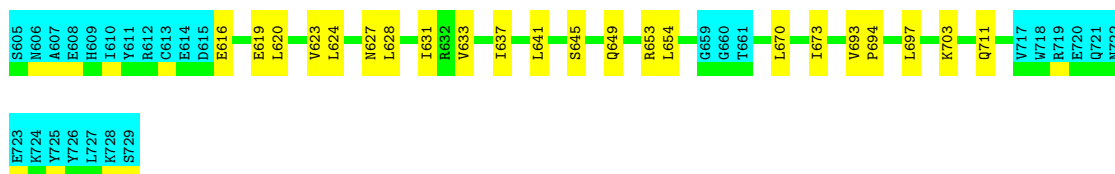


#### 4.2.5 Score per residue for model 5

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a

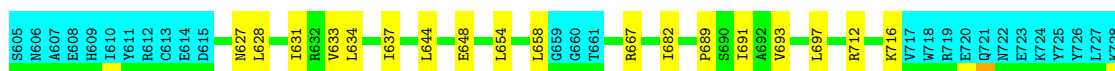


#### 4.2.6 Score per residue for model 6

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



S729

#### 4.2.7 Score per residue for model 7

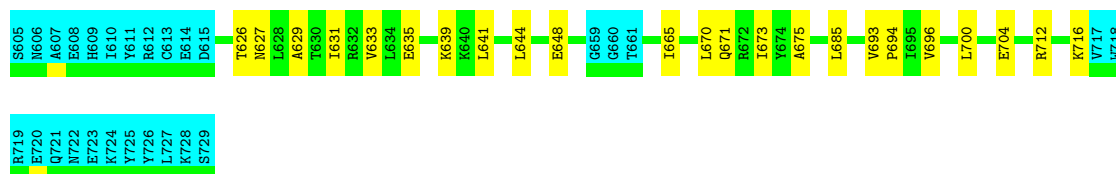
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 



#### 4.2.8 Score per residue for model 8


- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 



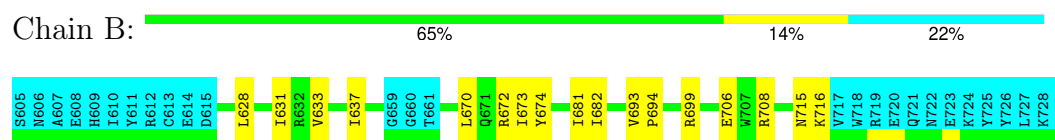
#### 4.2.9 Score per residue for model 9

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

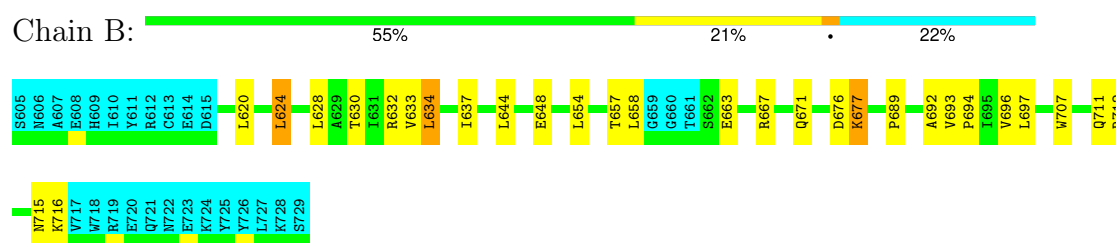


#### 4.2.10 Score per residue for model 10

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a

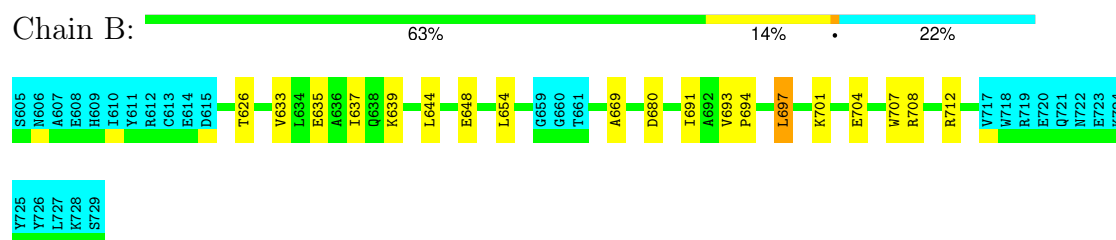


#### 4.2.11 Score per residue for model 11

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



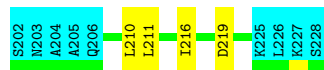
- Molecule 2: Paired amphipathic helix protein Sin3a



### 4.2.12 Score per residue for model 12

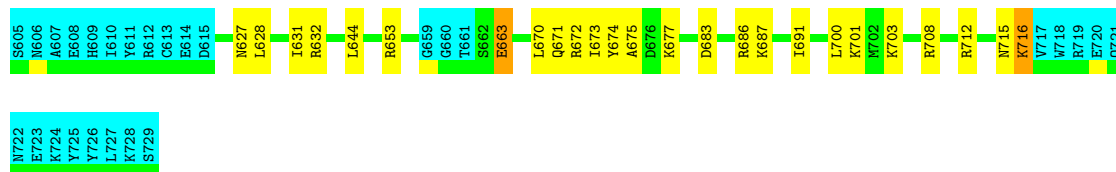
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

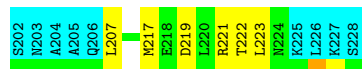
Chain B: 



### 4.2.13 Score per residue for model 13

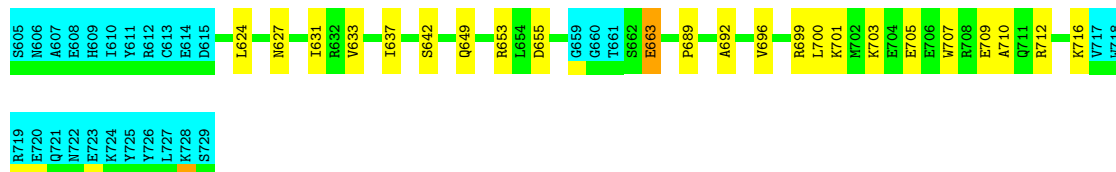
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 



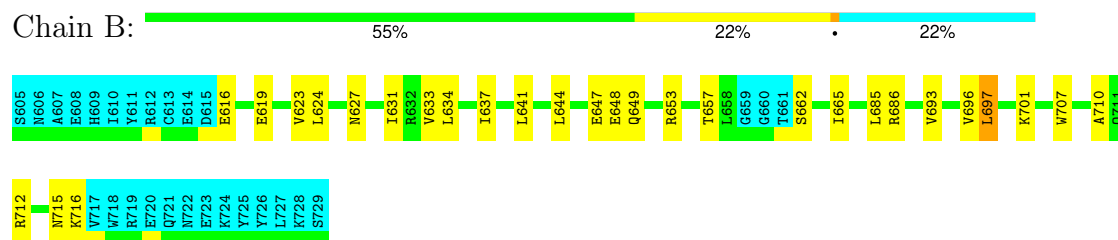
### 4.2.14 Score per residue for model 14

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

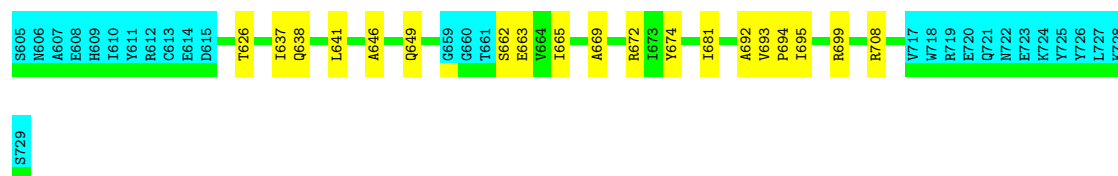


#### 4.2.15 Score per residue for model 15

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a

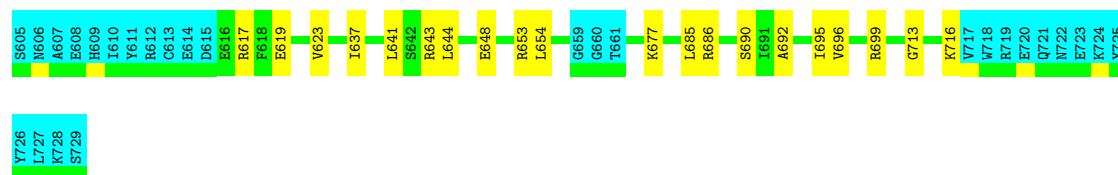


#### 4.2.16 Score per residue for model 16

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



### 4.2.17 Score per residue for model 17

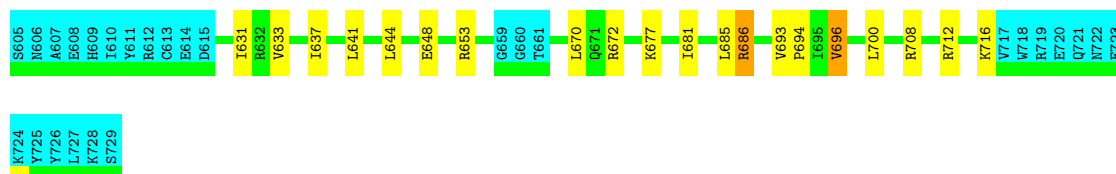
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 



### 4.2.18 Score per residue for model 18

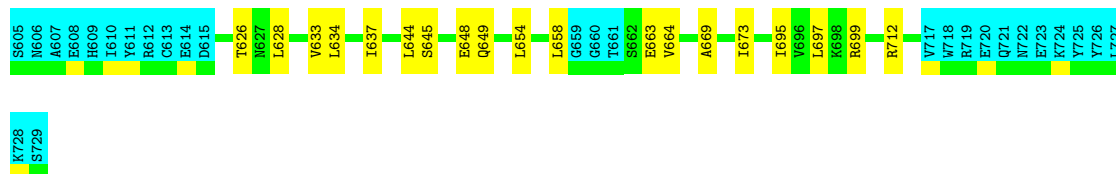
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

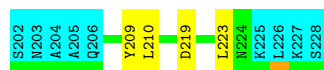
Chain B: 



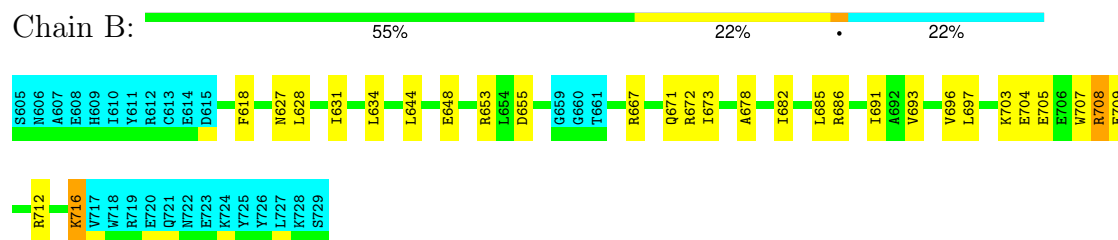
### 4.2.19 Score per residue for model 19

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

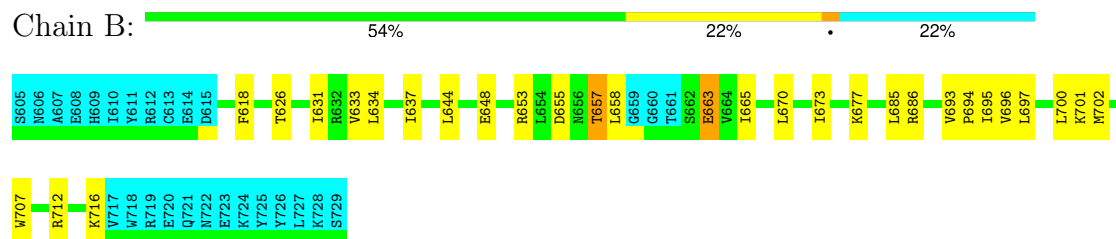


#### 4.2.20 Score per residue for model 20

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



## 5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| ARIA          | structure solution |         |
| CNS           | 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               | 2              |
| Total number of shifts                       | 1790           |
| Number of shifts mapped to atoms             | 1790           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 83%            |

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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     | 152   | 151      | 151      | 2±1     |
| 2   | B     | 803   | 850      | 849      | 12±4    |
| All | All   | 19100 | 20020    | 20000    | 269     |

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 7.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:634:LEU:HB3  | 2:B:697:LEU:HD13 | 0.81     | 1.50        | 20     | 5     |
| 2:B:634:LEU:HB3  | 2:B:697:LEU:HG   | 0.68     | 1.64        | 6      | 3     |
| 1:A:216:ILE:HG21 | 2:B:677:LYS:HB3  | 0.67     | 1.65        | 12     | 1     |
| 2:B:685:LEU:HD21 | 2:B:696:VAL:HG21 | 0.65     | 1.67        | 19     | 5     |
| 2:B:670:LEU:HD23 | 2:B:682:ILE:HG12 | 0.64     | 1.69        | 9      | 1     |
| 2:B:712:ARG:HA   | 2:B:716:LYS:HB3  | 0.61     | 1.72        | 4      | 4     |
| 2:B:644:LEU:HB3  | 2:B:648:GLU:HB2  | 0.61     | 1.73        | 10     | 11    |
| 2:B:667:ARG:HG3  | 2:B:682:ILE:HG12 | 0.59     | 1.72        | 19     | 1     |
| 2:B:635:GLU:O    | 2:B:639:LYS:HG2  | 0.59     | 1.97        | 11     | 1     |
| 2:B:704:GLU:O    | 2:B:708:ARG:HG2  | 0.58     | 1.98        | 4      | 2     |
| 2:B:683:ASP:OD2  | 2:B:687:LYS:HE2  | 0.58     | 1.98        | 12     | 1     |
| 2:B:633:VAL:O    | 2:B:637:ILE:HG12 | 0.57     | 1.99        | 6      | 11    |
| 1:A:209:TYR:HB3  | 2:B:672:ARG:HD2  | 0.56     | 1.76        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:654:LEU:HD23 | 2:B:658:LEU:HD21 | 0.56     | 1.78        | 2      | 1     |
| 2:B:619:GLU:O    | 2:B:623:VAL:HG23 | 0.56     | 2.00        | 5      | 2     |
| 2:B:641:LEU:O    | 2:B:644:LEU:HG   | 0.55     | 2.01        | 2      | 3     |
| 2:B:673:ILE:HG21 | 2:B:703:LYS:HG3  | 0.55     | 1.76        | 19     | 1     |
| 2:B:667:ARG:O    | 2:B:671:GLN:HG3  | 0.55     | 2.01        | 19     | 2     |
| 1:A:219:ASP:O    | 1:A:223:LEU:HG   | 0.54     | 2.01        | 19     | 9     |
| 1:A:217:MET:SD   | 2:B:677:LYS:HE2  | 0.54     | 2.41        | 16     | 1     |
| 1:A:216:ILE:O    | 1:A:220:LEU:HB2  | 0.54     | 2.02        | 9      | 1     |
| 2:B:674:TYR:CD1  | 2:B:681:ILE:HG13 | 0.54     | 2.37        | 9      | 2     |
| 1:A:211:LEU:HG   | 2:B:673:ILE:HB   | 0.54     | 1.79        | 9      | 1     |
| 2:B:671:GLN:O    | 2:B:675:ALA:HA   | 0.54     | 2.03        | 7      | 2     |
| 1:A:211:LEU:HD21 | 2:B:703:LYS:HD2  | 0.53     | 1.80        | 12     | 1     |
| 2:B:673:ILE:HG21 | 2:B:703:LYS:HG2  | 0.53     | 1.79        | 2      | 1     |
| 2:B:653:ARG:HD2  | 2:B:686:ARG:O    | 0.53     | 2.04        | 2      | 4     |
| 2:B:693:VAL:HB   | 2:B:694:PRO:HD3  | 0.53     | 1.80        | 20     | 7     |
| 2:B:643:ARG:HA   | 2:B:690:SER:OG   | 0.53     | 2.03        | 16     | 1     |
| 2:B:634:LEU:CB   | 2:B:697:LEU:HD13 | 0.53     | 2.33        | 2      | 1     |
| 1:A:220:LEU:HD11 | 2:B:677:LYS:HG2  | 0.53     | 1.80        | 20     | 1     |
| 2:B:654:LEU:HA   | 2:B:657:THR:OG1  | 0.52     | 2.03        | 3      | 1     |
| 2:B:631:ILE:CD1  | 2:B:700:LEU:HB3  | 0.52     | 2.35        | 13     | 2     |
| 2:B:712:ARG:HA   | 2:B:716:LYS:CB   | 0.52     | 2.33        | 6      | 4     |
| 2:B:693:VAL:O    | 2:B:697:LEU:HB2  | 0.52     | 2.05        | 11     | 4     |
| 2:B:674:TYR:OH   | 2:B:699:ARG:HG3  | 0.52     | 2.05        | 9      | 2     |
| 2:B:708:ARG:O    | 2:B:712:ARG:HB2  | 0.52     | 2.03        | 11     | 1     |
| 2:B:629:ALA:O    | 2:B:633:VAL:HG23 | 0.51     | 2.05        | 4      | 2     |
| 2:B:634:LEU:HD13 | 2:B:693:VAL:HG13 | 0.51     | 1.81        | 4      | 1     |
| 2:B:627:ASN:O    | 2:B:631:ILE:HG12 | 0.51     | 2.06        | 13     | 8     |
| 1:A:209:TYR:HD2  | 2:B:707:TRP:HE1  | 0.51     | 1.49        | 11     | 1     |
| 2:B:631:ILE:HD13 | 2:B:700:LEU:HB3  | 0.51     | 1.83        | 4      | 2     |
| 2:B:695:ILE:O    | 2:B:699:ARG:HG2  | 0.51     | 2.06        | 18     | 5     |
| 2:B:637:ILE:O    | 2:B:641:LEU:HG   | 0.51     | 2.06        | 16     | 7     |
| 2:B:708:ARG:O    | 2:B:712:ARG:HG2  | 0.50     | 2.05        | 1      | 1     |
| 2:B:654:LEU:HD12 | 2:B:658:LEU:HD13 | 0.50     | 1.81        | 18     | 1     |
| 2:B:671:GLN:HG2  | 2:B:678:ALA:HB1  | 0.50     | 1.81        | 19     | 1     |
| 2:B:654:LEU:CD1  | 2:B:689:PRO:HB3  | 0.50     | 2.36        | 10     | 2     |
| 2:B:685:LEU:HD21 | 2:B:696:VAL:HG11 | 0.50     | 1.83        | 17     | 4     |
| 2:B:658:LEU:HB2  | 2:B:663:GLU:HG3  | 0.50     | 1.82        | 10     | 1     |
| 2:B:672:ARG:HA   | 2:B:672:ARG:NE   | 0.50     | 2.22        | 9      | 1     |
| 2:B:663:GLU:OE2  | 2:B:667:ARG:HB2  | 0.50     | 2.07        | 4      | 1     |
| 2:B:692:ALA:O    | 2:B:696:VAL:HG22 | 0.50     | 2.07        | 4      | 4     |
| 2:B:662:SER:HB2  | 2:B:665:ILE:HB   | 0.50     | 1.82        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:629:ALA:HA   | 2:B:632:ARG:HH21 | 0.50     | 1.67        | 4      | 1     |
| 2:B:693:VAL:HG12 | 2:B:694:PRO:HD3  | 0.50     | 1.83        | 7      | 1     |
| 2:B:712:ARG:O    | 2:B:716:LYS:HB3  | 0.50     | 2.06        | 17     | 2     |
| 2:B:626:THR:HG22 | 2:B:669:ALA:HB2  | 0.49     | 1.84        | 15     | 3     |
| 2:B:697:LEU:O    | 2:B:701:LYS:HG2  | 0.49     | 2.07        | 1      | 3     |
| 2:B:663:GLU:O    | 2:B:667:ARG:HD3  | 0.49     | 2.06        | 3      | 1     |
| 2:B:653:ARG:HG3  | 2:B:689:PRO:HD3  | 0.49     | 1.84        | 4      | 1     |
| 2:B:704:GLU:O    | 2:B:708:ARG:HB2  | 0.49     | 2.07        | 19     | 1     |
| 2:B:626:THR:HG23 | 2:B:665:ILE:HB   | 0.49     | 1.83        | 7      | 3     |
| 2:B:712:ARG:HA   | 2:B:716:LYS:CG   | 0.49     | 2.37        | 8      | 1     |
| 1:A:211:LEU:HB2  | 2:B:673:ILE:HB   | 0.49     | 1.81        | 3      | 2     |
| 2:B:649:GLN:O    | 2:B:653:ARG:HB2  | 0.48     | 2.07        | 5      | 1     |
| 2:B:673:ILE:HG13 | 2:B:674:TYR:CD2  | 0.48     | 2.42        | 12     | 1     |
| 2:B:712:ARG:HA   | 2:B:716:LYS:HB2  | 0.48     | 1.84        | 19     | 3     |
| 2:B:711:GLN:HG3  | 2:B:715:ASN:HB3  | 0.48     | 1.86        | 2      | 1     |
| 2:B:637:ILE:HG21 | 2:B:654:LEU:HD21 | 0.48     | 1.84        | 5      | 4     |
| 1:A:208:ASN:HB2  | 2:B:706:GLU:OE2  | 0.48     | 2.09        | 9      | 1     |
| 2:B:636:ALA:O    | 2:B:640:LYS:HG2  | 0.48     | 2.07        | 3      | 1     |
| 1:A:223:LEU:CD2  | 2:B:692:ALA:HA   | 0.47     | 2.38        | 1      | 3     |
| 2:B:689:PRO:O    | 2:B:693:VAL:HB   | 0.47     | 2.09        | 6      | 1     |
| 1:A:217:MET:O    | 1:A:221:ARG:HG3  | 0.47     | 2.09        | 13     | 1     |
| 1:A:216:ILE:HG21 | 2:B:677:LYS:HB2  | 0.47     | 1.85        | 16     | 1     |
| 1:A:223:LEU:HD23 | 2:B:695:ILE:HD12 | 0.47     | 1.85        | 16     | 2     |
| 2:B:628:LEU:O    | 2:B:632:ARG:HG2  | 0.47     | 2.09        | 12     | 1     |
| 1:A:217:MET:O    | 1:A:221:ARG:HG2  | 0.47     | 2.10        | 15     | 3     |
| 1:A:221:ARG:HA   | 1:A:221:ARG:HE   | 0.46     | 1.71        | 8      | 1     |
| 2:B:673:ILE:HG22 | 2:B:703:LYS:HG3  | 0.46     | 1.86        | 5      | 1     |
| 2:B:712:ARG:HG3  | 2:B:716:LYS:HD3  | 0.46     | 1.86        | 13     | 1     |
| 2:B:635:GLU:O    | 2:B:639:LYS:HG3  | 0.46     | 2.10        | 7      | 1     |
| 2:B:624:LEU:CD2  | 2:B:707:TRP:HB3  | 0.46     | 2.41        | 13     | 2     |
| 2:B:667:ARG:HG3  | 2:B:682:ILE:HD13 | 0.45     | 1.88        | 6      | 1     |
| 1:A:209:TYR:HD1  | 2:B:707:TRP:HE1  | 0.45     | 1.55        | 19     | 2     |
| 2:B:634:LEU:CD1  | 2:B:693:VAL:HG13 | 0.45     | 2.42        | 4      | 1     |
| 2:B:620:LEU:HB3  | 2:B:711:GLN:OE1  | 0.45     | 2.12        | 10     | 1     |
| 2:B:653:ARG:HG3  | 2:B:686:ARG:O    | 0.45     | 2.12        | 17     | 1     |
| 1:A:210:LEU:HA   | 2:B:672:ARG:O    | 0.45     | 2.12        | 12     | 1     |
| 2:B:654:LEU:HD22 | 2:B:658:LEU:HD13 | 0.44     | 1.87        | 4      | 1     |
| 2:B:670:LEU:HD12 | 2:B:673:ILE:HD11 | 0.44     | 1.89        | 7      | 2     |
| 2:B:678:ALA:O    | 2:B:682:ILE:HG12 | 0.44     | 2.12        | 8      | 2     |
| 2:B:644:LEU:HD22 | 2:B:648:GLU:HB3  | 0.44     | 1.88        | 11     | 1     |
| 2:B:624:LEU:HG   | 2:B:711:GLN:HG2  | 0.44     | 1.88        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:694:PRO:O    | 2:B:698:LYS:HG3  | 0.44     | 2.13        | 3      | 1     |
| 2:B:662:SER:HB3  | 2:B:665:ILE:HD11 | 0.44     | 1.89        | 14     | 1     |
| 2:B:631:ILE:HD11 | 2:B:700:LEU:HG   | 0.44     | 1.89        | 17     | 1     |
| 2:B:677:LYS:O    | 2:B:681:ILE:HG12 | 0.44     | 2.13        | 17     | 1     |
| 2:B:644:LEU:HB3  | 2:B:648:GLU:CB   | 0.44     | 2.43        | 20     | 1     |
| 2:B:653:ARG:HD2  | 2:B:655:ASP:OD1  | 0.44     | 2.12        | 13     | 1     |
| 1:A:216:ILE:HG12 | 2:B:674:TYR:HD1  | 0.44     | 1.73        | 1      | 1     |
| 1:A:210:LEU:HD23 | 2:B:672:ARG:O    | 0.44     | 2.12        | 19     | 1     |
| 2:B:705:GLU:O    | 2:B:709:GLU:HG2  | 0.43     | 2.13        | 13     | 2     |
| 2:B:701:LYS:O    | 2:B:704:GLU:HB3  | 0.43     | 2.14        | 11     | 1     |
| 2:B:619:GLU:O    | 2:B:623:VAL:HG12 | 0.43     | 2.12        | 14     | 1     |
| 2:B:633:VAL:O    | 2:B:637:ILE:HG13 | 0.43     | 2.14        | 17     | 1     |
| 1:A:214:GLU:O    | 1:A:218:GLU:HB2  | 0.43     | 2.14        | 4      | 1     |
| 2:B:646:ALA:HA   | 2:B:649:GLN:HE21 | 0.43     | 1.74        | 15     | 1     |
| 2:B:702:MET:O    | 2:B:705:GLU:HB2  | 0.43     | 2.14        | 3      | 1     |
| 2:B:631:ILE:CD1  | 2:B:700:LEU:HG   | 0.43     | 2.43        | 2      | 4     |
| 1:A:221:ARG:NE   | 1:A:221:ARG:HA   | 0.43     | 2.28        | 6      | 1     |
| 1:A:210:LEU:HD13 | 2:B:672:ARG:O    | 0.43     | 2.14        | 15     | 1     |
| 1:A:211:LEU:HB2  | 2:B:673:ILE:O    | 0.43     | 2.13        | 18     | 1     |
| 2:B:649:GLN:OE1  | 2:B:689:PRO:HG2  | 0.42     | 2.14        | 2      | 1     |
| 2:B:654:LEU:HG   | 2:B:658:LEU:HD12 | 0.42     | 1.89        | 6      | 1     |
| 2:B:629:ALA:HA   | 2:B:632:ARG:NH2  | 0.42     | 2.29        | 4      | 1     |
| 2:B:634:LEU:HB3  | 2:B:697:LEU:HD23 | 0.42     | 1.91        | 4      | 1     |
| 2:B:624:LEU:HG   | 2:B:711:GLN:OE1  | 0.42     | 2.14        | 5      | 1     |
| 2:B:645:SER:O    | 2:B:649:GLN:HG3  | 0.42     | 2.14        | 18     | 2     |
| 2:B:654:LEU:HD12 | 2:B:654:LEU:N    | 0.42     | 2.29        | 2      | 1     |
| 2:B:653:ARG:HA   | 2:B:689:PRO:HG3  | 0.42     | 1.90        | 4      | 1     |
| 2:B:632:ARG:HA   | 2:B:632:ARG:NE   | 0.42     | 2.29        | 3      | 1     |
| 1:A:207:LEU:HD23 | 2:B:710:ALA:HB1  | 0.42     | 1.91        | 13     | 1     |
| 1:A:209:TYR:O    | 2:B:673:ILE:HG22 | 0.42     | 2.15        | 20     | 1     |
| 2:B:693:VAL:HA   | 2:B:696:VAL:HG22 | 0.42     | 1.91        | 19     | 1     |
| 2:B:673:ILE:CG2  | 2:B:703:LYS:HG3  | 0.42     | 2.45        | 5      | 1     |
| 2:B:707:TRP:O    | 2:B:711:GLN:HB2  | 0.42     | 2.15        | 10     | 1     |
| 2:B:649:GLN:HB3  | 2:B:689:PRO:HG2  | 0.41     | 1.90        | 13     | 1     |
| 1:A:216:ILE:HG12 | 2:B:674:TYR:CD1  | 0.41     | 2.51        | 1      | 1     |
| 2:B:630:THR:O    | 2:B:634:LEU:HB2  | 0.41     | 2.15        | 10     | 1     |
| 2:B:653:ARG:HD3  | 2:B:686:ARG:O    | 0.41     | 2.16        | 20     | 2     |
| 2:B:676:ASP:OD1  | 2:B:677:LYS:HG2  | 0.41     | 2.16        | 10     | 1     |
| 1:A:207:LEU:HB3  | 1:A:209:TYR:CE2  | 0.41     | 2.49        | 7      | 1     |
| 1:A:224:ASN:HD22 | 1:A:224:ASN:N    | 0.41     | 2.13        | 2      | 1     |
| 2:B:634:LEU:HD12 | 2:B:697:LEU:HB2  | 0.41     | 1.91        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:627:ASN:OD1  | 2:B:704:GLU:HA   | 0.41     | 2.16        | 7      | 1     |
| 2:B:709:GLU:O    | 2:B:712:ARG:HG2  | 0.41     | 2.15        | 8      | 1     |
| 2:B:647:GLU:H    | 2:B:647:GLU:CD   | 0.41     | 2.19        | 14     | 1     |
| 1:A:213:ASP:O    | 1:A:217:MET:HG3  | 0.41     | 2.15        | 15     | 1     |
| 2:B:693:VAL:N    | 2:B:694:PRO:HD2  | 0.41     | 2.31        | 15     | 2     |
| 2:B:711:GLN:NE2  | 2:B:715:ASN:HB2  | 0.41     | 2.31        | 10     | 1     |
| 2:B:657:THR:HB   | 2:B:658:LEU:HD12 | 0.41     | 1.93        | 20     | 1     |
| 2:B:620:LEU:O    | 2:B:624:LEU:HD23 | 0.41     | 2.16        | 5      | 1     |
| 2:B:628:LEU:O    | 2:B:632:ARG:HG3  | 0.40     | 2.17        | 10     | 1     |
| 2:B:641:LEU:HD22 | 2:B:649:GLN:OE1  | 0.40     | 2.17        | 14     | 1     |
| 2:B:645:SER:O    | 2:B:649:GLN:HG2  | 0.40     | 2.17        | 2      | 1     |
| 2:B:687:LYS:HZ3  | 2:B:687:LYS:HB2  | 0.40     | 1.76        | 4      | 1     |
| 2:B:663:GLU:HG3  | 2:B:664:VAL:N    | 0.40     | 2.32        | 18     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1   | A     | 18/27 (67%)     | 17±1 (96±4%) | 1±1 (4±4%) | 0±0 (0±0%) | 100         | 100 |
| 2   | B     | 98/125 (78%)    | 91±2 (93±2%) | 7±2 (7±2%) | 0±0 (0±0%) | 45          | 81  |
| All | All   | 2320/3040 (76%) | 2171 (94%)   | 146 (6%)   | 3 (0%)     | 50          | 84  |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 655 | ASP  | 2              |
| 2   | B     | 642 | SER  | 1              |

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 18/25 (72%)     | 17±1 (96±5%) | 1±1 (4±5%) | 30          | 82 |
| 2   | B     | 86/110 (78%)    | 83±2 (97±2%) | 3±2 (3±2%) | 35          | 86 |
| All | All   | 2080/2700 (77%) | 2010 (97%)   | 70 (3%)    | 34          | 85 |

All 33 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) |
|-----|-------|-----|------|----------------|
| 2   | B     | 708 | ARG  | 6              |
| 2   | B     | 657 | THR  | 5              |
| 1   | A     | 224 | ASN  | 5              |
| 2   | B     | 628 | LEU  | 5              |
| 2   | B     | 663 | GLU  | 4              |
| 2   | B     | 638 | GLN  | 3              |
| 2   | B     | 701 | LYS  | 3              |
| 2   | B     | 670 | LEU  | 3              |
| 2   | B     | 716 | LYS  | 3              |
| 2   | B     | 617 | ARG  | 2              |
| 2   | B     | 677 | LYS  | 2              |
| 2   | B     | 702 | MET  | 2              |
| 2   | B     | 634 | LEU  | 2              |
| 1   | A     | 219 | ASP  | 2              |
| 1   | A     | 217 | MET  | 2              |
| 2   | B     | 697 | LEU  | 2              |
| 2   | B     | 715 | ASN  | 2              |
| 2   | B     | 699 | ARG  | 2              |
| 2   | B     | 639 | LYS  | 1              |
| 1   | A     | 213 | ASP  | 1              |
| 2   | B     | 687 | LYS  | 1              |
| 2   | B     | 705 | GLU  | 1              |
| 1   | A     | 220 | LEU  | 1              |
| 2   | B     | 631 | ILE  | 1              |
| 2   | B     | 624 | LEU  | 1              |
| 2   | B     | 680 | ASP  | 1              |
| 2   | B     | 644 | LEU  | 1              |
| 2   | B     | 703 | LYS  | 1              |
| 1   | A     | 211 | LEU  | 1              |
| 1   | A     | 218 | GLU  | 1              |
| 1   | A     | 207 | LEU  | 1              |
| 2   | B     | 686 | ARG  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 696 | VAL  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|   |      |
|---|------|
| Total number of shifts                  | 1518 |
| Number of shifts mapped to atoms        | 1518 |
| 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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 125      | $-0.59 \pm 0.10$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 121      | $0.02 \pm 0.09$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 122      | $-0.44 \pm 0.09$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 116      | $0.65 \pm 0.28$                 | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 1225 atoms were assigned a chemical shift out of a possible 1724. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 480/578 (83%)  | 193/232 (83%) | 195/232 (84%)   | 92/114 (81%)    |
| Sidechain | 718/1078 (67%) | 476/695 (68%) | 234/329 (71%)   | 8/54 (15%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 27/68 (40%)     | 14/33 (42%)    | 12/32 (38%)     | 1/3 (33%)       |
| Overall  | 1225/1724 (71%) | 683/960 (71%)  | 441/593 (74%)   | 101/171 (59%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1518 atoms were assigned a chemical shift out of a possible 2211. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 607/760 (80%)   | 244/306 (80%)  | 247/304 (81%)   | 116/150 (77%)   |
| Sidechain | 858/1336 (64%)  | 564/858 (66%)  | 283/409 (69%)   | 11/69 (16%)     |
| Aromatic  | 53/115 (46%)    | 27/55 (49%)    | 24/54 (44%)     | 2/6 (33%)       |
| Overall   | 1518/2211 (69%) | 835/1219 (68%) | 554/767 (72%)   | 129/225 (57%)   |

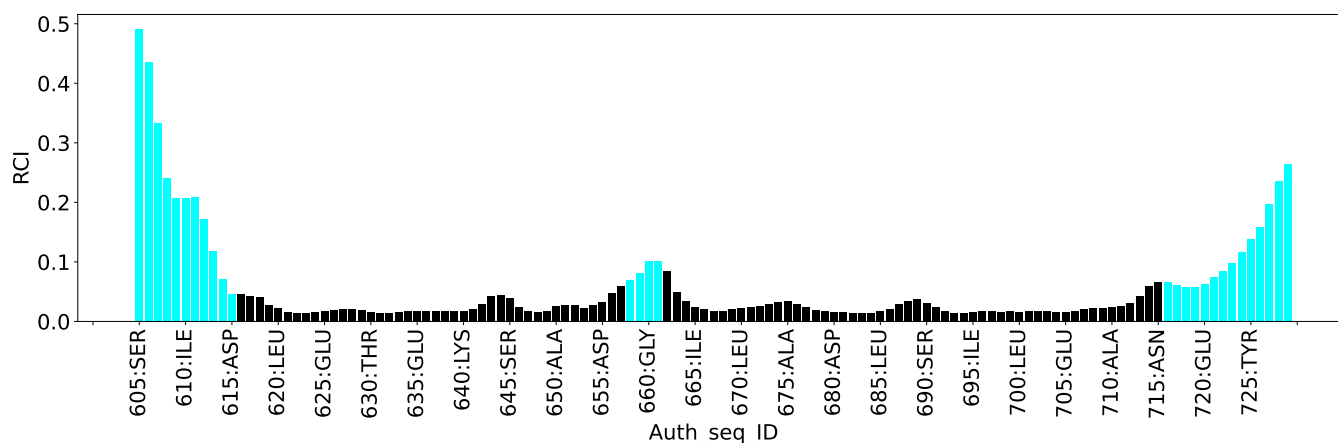
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain B:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 Bookkeeping

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

|   |     |
|---|-----|
| Total number of shifts                  | 272 |
| Number of shifts mapped to atoms        | 272 |
| 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   |

### 7.2.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 12%, i.e. 207 atoms were assigned a chemical shift out of a possible 1724. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 69/578 (12%)   | 35/232 (15%)         | 17/232 (7%)           | 17/114 (15%)          |
| Sidechain | 136/1078 (13%) | 93/695 (13%)         | 41/329 (12%)          | 2/54 (4%)             |
| Aromatic  | 2/68 (3%)      | 2/33 (6%)            | 0/32 (0%)             | 0/3 (0%)              |
| Overall   | 207/1724 (12%) | 130/960 (14%)        | 58/593 (10%)          | 19/171 (11%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 272 atoms were assigned a chemical shift out of a possible 2211. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 93/760 (12%)   | 48/306 (16%)         | 22/304 (7%)           | 23/150 (15%)          |
| Sidechain | 177/1336 (13%) | 120/858 (14%)        | 55/409 (13%)          | 2/69 (3%)             |
| Aromatic  | 2/115 (2%)     | 2/55 (4%)            | 0/54 (0%)             | 0/6 (0%)              |
| Overall   | 272/2211 (12%) | 170/1219 (14%)       | 77/767 (10%)          | 25/225 (11%)          |

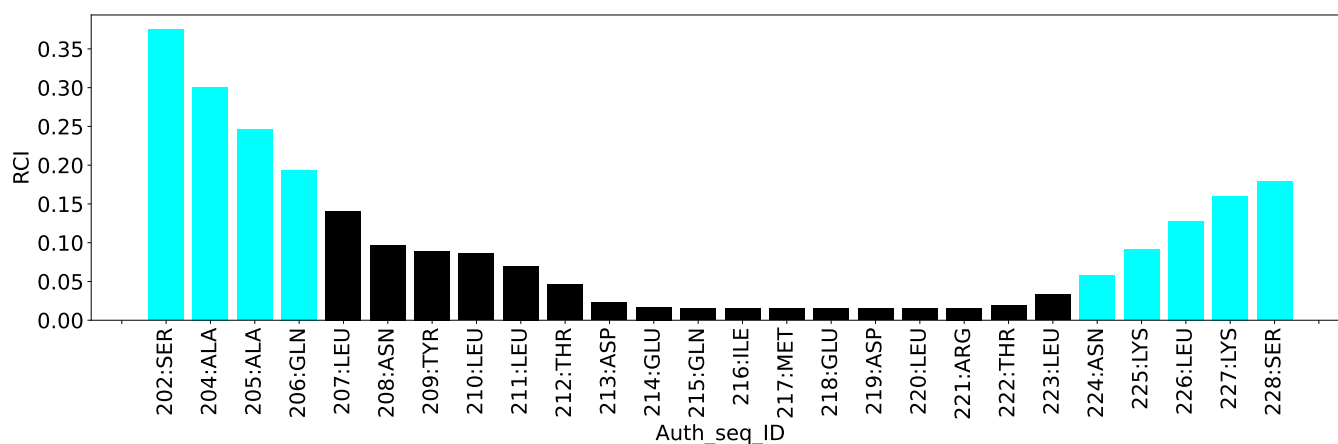
## 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description  | Value |
|--|-------|
| Total distance restraints                                | 3007  |
| Intra-residue ( $ i-j =0$ )                              | 1388  |
| Sequential ( $ i-j =1$ )                                 | 560   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 468   |
| Long range ( $ i-j \geq 5$ )                             | 269   |
| Inter-chain  | 208   |
| Hydrogen bond restraints                                 | 114   |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 200   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 21.1  |
| Number of long range restraints per residue <sup>1</sup> | 1.8   |

<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)  | 37.5                                   | 0.2     |
| 0.2-0.5 (Medium) | 59.9                                   | 0.5     |
| >0.5 (Large)     | 42.8                                   | 3.25    |

### 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)   | 2.4                                    | 4.4     |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

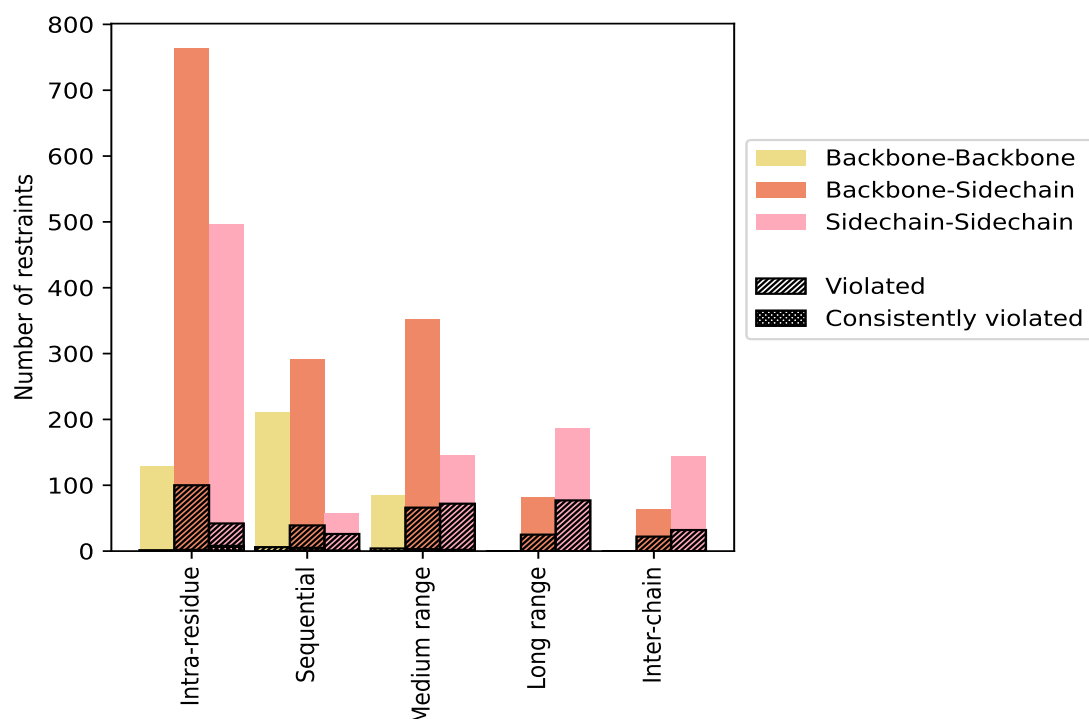
### 9.1 Summary of distance violations ⓘ

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

| Restraints type   | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|   |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>1388</b> | <b>46.2</b>    | <b>143</b>            | <b>10.3</b>    | <b>4.8</b>     | <b>11</b>                          | <b>0.8</b>     | <b>0.4</b>     |
| Backbone-Backbone   | 129         | 4.3            | 1                     | 0.8            | 0.0            | 1                                  | 0.8            | 0.0            |
| Backbone-Sidechain  | 763         | 25.4           | 100                   | 13.1           | 3.3            | 2                                  | 0.3            | 0.1            |
| Sidechain-Sidechain   | 496         | 16.5           | 42                    | 8.5            | 1.4            | 8                                  | 1.6            | 0.3            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>560</b>  | <b>18.6</b>    | <b>71</b>             | <b>12.7</b>    | <b>2.4</b>     | <b>6</b>                           | <b>1.1</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 211         | 7.0            | 6                     | 2.8            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 291         | 9.7            | 39                    | 13.4           | 1.3            | 5                                  | 1.7            | 0.2            |
| Sidechain-Sidechain   | 58          | 1.9            | 26                    | 44.8           | 0.9            | 1                                  | 1.7            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>468</b>  | <b>15.6</b>    | <b>133</b>            | <b>28.4</b>    | <b>4.4</b>     | <b>5</b>                           | <b>1.1</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 85          | 2.8            | 4                     | 4.7            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 238         | 7.9            | 57                    | 23.9           | 1.9            | 3                                  | 1.3            | 0.1            |
| Sidechain-Sidechain   | 145         | 4.8            | 72                    | 49.7           | 2.4            | 2                                  | 1.4            | 0.1            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>269</b>  | <b>8.9</b>     | <b>102</b>            | <b>37.9</b>    | <b>3.4</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 1           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 81          | 2.7            | 25                    | 30.9           | 0.8            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 187         | 6.2            | 77                    | 41.2           | 2.6            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>  | <b>208</b>  | <b>6.9</b>     | <b>54</b>             | <b>26.0</b>    | <b>1.8</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 1           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 63          | 2.1            | 22                    | 34.9           | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 144         | 4.8            | 32                    | 22.2           | 1.1            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>  | <b>114</b>  | <b>3.8</b>     | <b>9</b>              | <b>7.9</b>     | <b>0.3</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>   | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>  | <b>3007</b> | <b>100.0</b>   | <b>512</b>            | <b>17.0</b>    | <b>17.0</b>    | <b>22</b>                          | <b>0.7</b>     | <b>0.7</b>     |
| Backbone-Backbone   | 427         | 14.2           | 11                    | 2.6            | 0.4            | 1                                  | 0.2            | 0.0            |
| Backbone-Sidechain  | 1550        | 51.5           | 252                   | 16.3           | 8.4            | 10                                 | 0.6            | 0.3            |
| Sidechain-Sidechain   | 1030        | 34.3           | 249                   | 24.2           | 8.3            | 11                                 | 1.1            | 0.4            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 39                   | 21              | 31              | 27              | 12              | 130   | 0.4      | 1.77    | 0.31                | 0.3        |
| 2        | 33                   | 28              | 37              | 36              | 12              | 146   | 0.46     | 2.62    | 0.44                | 0.32       |
| 3        | 46                   | 19              | 43              | 32              | 13              | 153   | 0.47     | 1.85    | 0.37                | 0.33       |
| 4        | 45                   | 22              | 43              | 45              | 16              | 171   | 0.5      | 2.38    | 0.43                | 0.35       |
| 5        | 49                   | 24              | 41              | 38              | 13              | 165   | 0.52     | 2.27    | 0.4                 | 0.42       |
| 6        | 41                   | 21              | 40              | 35              | 10              | 147   | 0.47     | 1.68    | 0.37                | 0.35       |
| 7        | 43                   | 28              | 39              | 38              | 12              | 160   | 0.48     | 2.43    | 0.43                | 0.32       |
| 8        | 47                   | 27              | 37              | 39              | 7               | 157   | 0.45     | 2.46    | 0.37                | 0.32       |
| 9        | 38                   | 25              | 28              | 23              | 9               | 123   | 0.42     | 2.15    | 0.34                | 0.31       |
| 10       | 42                   | 19              | 41              | 27              | 14              | 143   | 0.48     | 2.51    | 0.43                | 0.33       |

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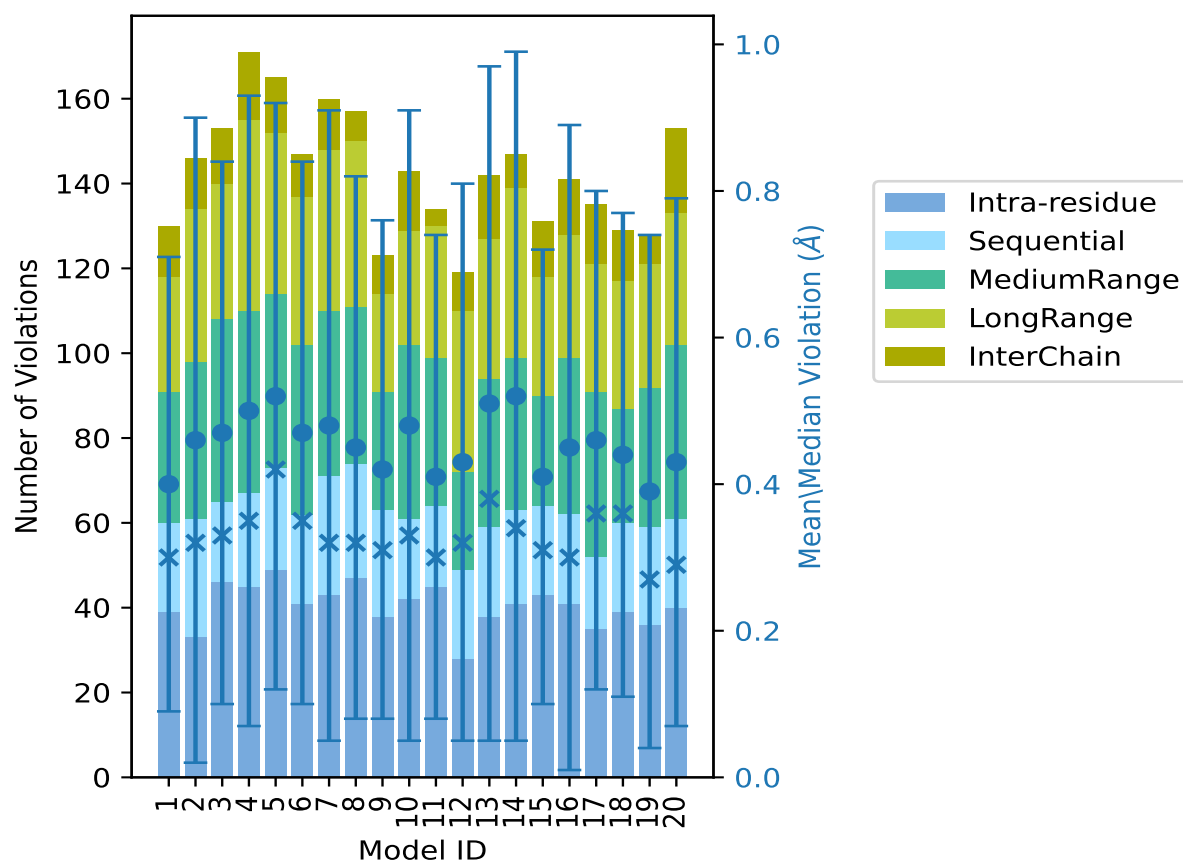
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 45                   | 19              | 35              | 31              | 4               | 134   | 0.41     | 1.71    | 0.33                | 0.3        |
| 12       | 28                   | 21              | 23              | 38              | 9               | 119   | 0.43     | 2.23    | 0.38                | 0.32       |
| 13       | 38                   | 21              | 35              | 33              | 15              | 142   | 0.51     | 3.13    | 0.46                | 0.38       |
| 14       | 41                   | 22              | 36              | 40              | 8               | 147   | 0.52     | 2.79    | 0.47                | 0.34       |
| 15       | 43                   | 21              | 26              | 28              | 13              | 131   | 0.41     | 1.41    | 0.31                | 0.31       |
| 16       | 41                   | 21              | 37              | 29              | 13              | 141   | 0.45     | 3.25    | 0.44                | 0.3        |
| 17       | 35                   | 17              | 39              | 30              | 14              | 135   | 0.46     | 2.17    | 0.34                | 0.36       |
| 18       | 39                   | 21              | 27              | 30              | 12              | 129   | 0.44     | 2.22    | 0.33                | 0.36       |
| 19       | 36                   | 23              | 33              | 29              | 7               | 128   | 0.39     | 2.23    | 0.35                | 0.27       |
| 20       | 40                   | 21              | 41              | 31              | 20              | 153   | 0.43     | 1.98    | 0.36                | 0.29       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

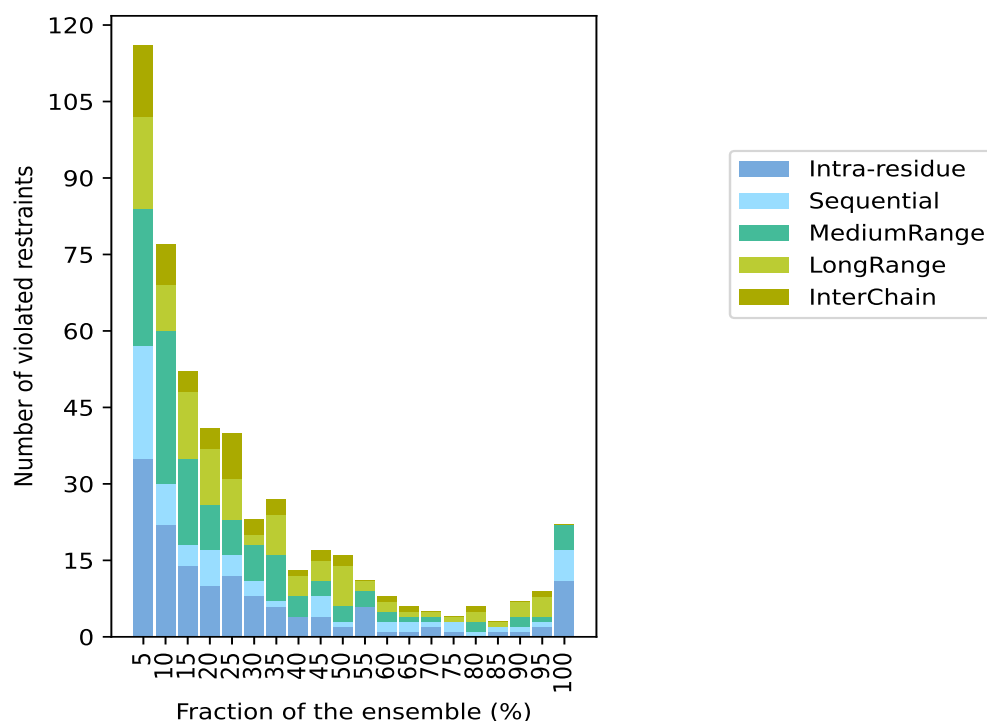
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2390(IR:1245, SQ:489, MR:335, LR:167, IC:154) restraints 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>       | %     |
| 35                            | 22              | 27              | 18              | 14              | 116   | 1                        | 5.0   |
| 22                            | 8               | 30              | 9               | 8               | 77    | 2                        | 10.0  |
| 14                            | 4               | 17              | 13              | 4               | 52    | 3                        | 15.0  |
| 10                            | 7               | 9               | 11              | 4               | 41    | 4                        | 20.0  |
| 12                            | 4               | 7               | 8               | 9               | 40    | 5                        | 25.0  |
| 8                             | 3               | 7               | 2               | 3               | 23    | 6                        | 30.0  |
| 6                             | 1               | 9               | 8               | 3               | 27    | 7                        | 35.0  |
| 4                             | 0               | 4               | 4               | 1               | 13    | 8                        | 40.0  |
| 4                             | 4               | 3               | 4               | 2               | 17    | 9                        | 45.0  |
| 2                             | 1               | 3               | 8               | 2               | 16    | 10                       | 50.0  |
| 6                             | 0               | 3               | 2               | 0               | 11    | 11                       | 55.0  |
| 1                             | 2               | 2               | 2               | 1               | 8     | 12                       | 60.0  |
| 1                             | 2               | 1               | 1               | 1               | 6     | 13                       | 65.0  |
| 2                             | 1               | 1               | 1               | 0               | 5     | 14                       | 70.0  |
| 1                             | 2               | 0               | 1               | 0               | 4     | 15                       | 75.0  |
| 0                             | 1               | 2               | 2               | 1               | 6     | 16                       | 80.0  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 17                       | 85.0  |
| 1                             | 1               | 2               | 3               | 0               | 7     | 18                       | 90.0  |
| 2                             | 1               | 1               | 4               | 1               | 9     | 19                       | 95.0  |
| 11                            | 6               | 5               | 0               | 0               | 22    | 20                       | 100.0 |

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

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

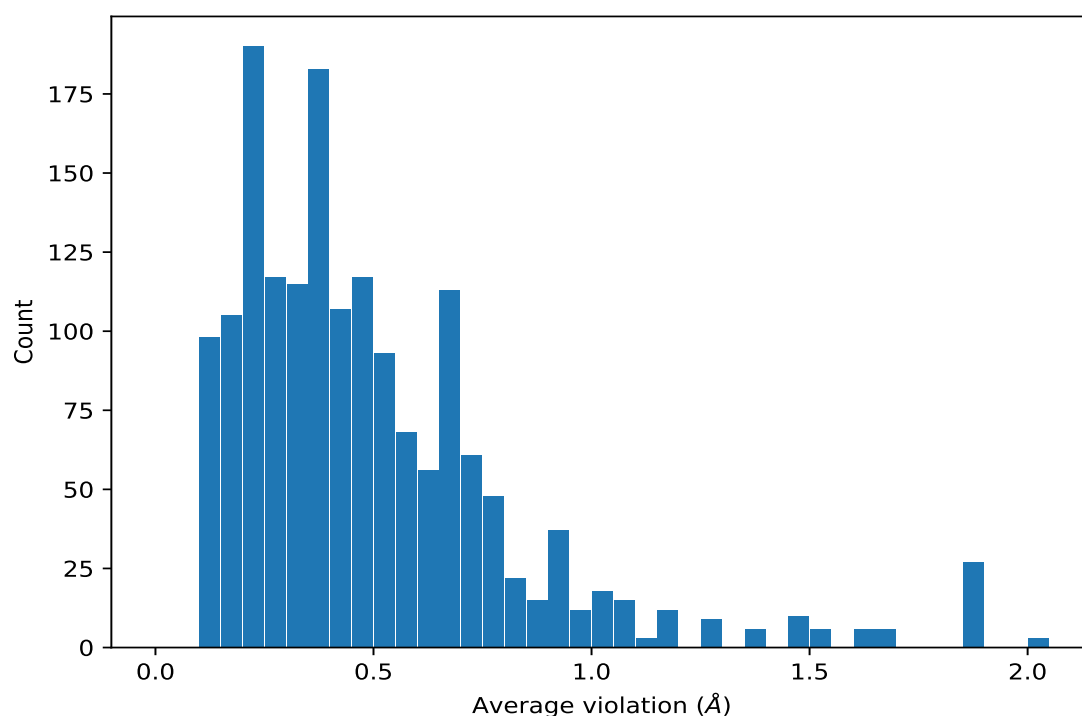
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 20                  | 0.94     | 0.17                | 0.94       |
| (1,750)  | 2:670:B:LEU:HB2  | 2:672:B:ARG:H    | 20                  | 0.94     | 0.17                | 0.94       |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 20                  | 0.93     | 0.16                | 0.99       |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 20                  | 0.93     | 0.16                | 0.99       |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 20                  | 0.8      | 0.37                | 0.72       |
| (1,210)  | 2:667:B:ARG:HB2  | 2:665:B:ILE:HG13 | 20                  | 0.8      | 0.37                | 0.72       |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 20                  | 0.76     | 0.09                | 0.77       |
| (1,1908) | 2:617:B:ARG:HG3  | 2:616:B:GLU:H    | 20                  | 0.76     | 0.09                | 0.77       |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 20                  | 0.65     | 0.42                | 0.55       |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 2:691:B:ILE:HG21 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 2:691:B:ILE:HG22 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 2:691:B:ILE:HG23 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 2:654:B:LEU:HD21 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,698)  | 2:654:B:LEU:HD22 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 2:654:B:LEU:HD23 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 1:223:A:LEU:HD11 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 1:223:A:LEU:HD12 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,698)  | 1:223:A:LEU:HD13 | 2:688:B:ASN:H    | 20                  | 0.5      | 0.26                | 0.39       |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 20                  | 0.46     | 0.13                | 0.42       |
| (1,672)  | 2:677:B:LYS:HG3  | 2:678:B:ALA:H    | 20                  | 0.46     | 0.13                | 0.42       |
| (1,672)  | 2:675:B:ALA:HB1  | 2:678:B:ALA:H    | 20                  | 0.46     | 0.13                | 0.42       |
| (1,672)  | 2:675:B:ALA:HB2  | 2:678:B:ALA:H    | 20                  | 0.46     | 0.13                | 0.42       |
| (1,672)  | 2:675:B:ALA:HB3  | 2:678:B:ALA:H    | 20                  | 0.46     | 0.13                | 0.42       |
| (1,672)  | 2:677:B:LYS:HD2  | 2:678:B:ALA:H    | 20                  | 0.46     | 0.13                | 0.42       |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 20                  | 0.44     | 0.31                | 0.35       |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 20                  | 0.44     | 0.31                | 0.35       |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 20                  | 0.44     | 0.31                | 0.35       |
| (1,1122) | 2:716:B:LYS:HB2  | 2:717:B:VAL:HG11 | 20                  | 0.44     | 0.31                | 0.35       |
| (1,1122) | 2:716:B:LYS:HB2  | 2:717:B:VAL:HG12 | 20                  | 0.44     | 0.31                | 0.35       |
| (1,1122) | 2:716:B:LYS:HB2  | 2:717:B:VAL:HG13 | 20                  | 0.44     | 0.31                | 0.35       |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 20                  | 0.44     | 0.04                | 0.44       |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 20                  | 0.44     | 0.04                | 0.44       |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 20                  | 0.44     | 0.04                | 0.44       |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 20                  | 0.43     | 0.13                | 0.42       |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 20                  | 0.43     | 0.03                | 0.44       |
| (1,740)  | 2:704:B:GLU:HG3  | 2:704:B:GLU:H    | 20                  | 0.43     | 0.03                | 0.44       |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 20                  | 0.29     | 0.06                | 0.28       |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 20                  | 0.25     | 0.09                | 0.27       |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG3  | 20                  | 0.25     | 0.09                | 0.27       |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 20                  | 0.25     | 0.09                | 0.25       |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 20                  | 0.25     | 0.09                | 0.25       |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 20                  | 0.25     | 0.09                | 0.25       |
| (1,226)  | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 20                  | 0.23     | 0.05                | 0.21       |
| (1,226)  | 2:608:B:GLU:HG3  | 2:608:B:GLU:HB3  | 20                  | 0.23     | 0.05                | 0.21       |
| (1,203)  | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 20                  | 0.21     | 0.02                | 0.21       |
| (1,203)  | 2:728:B:LYS:HD2  | 2:728:B:LYS:HG3  | 20                  | 0.21     | 0.02                | 0.21       |
| (1,203)  | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG3  | 20                  | 0.21     | 0.02                | 0.21       |
| (1,203)  | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 20                  | 0.21     | 0.02                | 0.21       |
| (1,203)  | 2:728:B:LYS:HD2  | 2:728:B:LYS:HG2  | 20                  | 0.21     | 0.02                | 0.21       |
| (1,220)  | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 20                  | 0.21     | 0.06                | 0.21       |
| (1,220)  | 2:647:B:GLU:HG3  | 2:647:B:GLU:HB3  | 20                  | 0.21     | 0.06                | 0.21       |
| (1,220)  | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 20                  | 0.21     | 0.06                | 0.21       |
| (1,220)  | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB2  | 20                  | 0.21     | 0.06                | 0.21       |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 20                  | 0.21     | 0.02                | 0.21       |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 20                  | 0.2      | 0.02                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG3  | 20                  | 0.2      | 0.02                | 0.2        |
| (1,223)  | 2:728:B:LYS:HG3  | 2:728:B:LYS:HD2  | 20                  | 0.2      | 0.03                | 0.21       |
| (1,223)  | 2:716:B:LYS:HG3  | 2:716:B:LYS:HD2  | 20                  | 0.2      | 0.03                | 0.21       |
| (1,223)  | 2:728:B:LYS:HG2  | 2:728:B:LYS:HD3  | 20                  | 0.2      | 0.03                | 0.21       |
| (1,223)  | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD2  | 20                  | 0.2      | 0.03                | 0.21       |
| (1,223)  | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD3  | 20                  | 0.2      | 0.03                | 0.21       |
| (1,403)  | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD2  | 20                  | 0.2      | 0.05                | 0.2        |
| (1,403)  | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 20                  | 0.2      | 0.05                | 0.2        |
| (1,403)  | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD3  | 20                  | 0.2      | 0.05                | 0.2        |
| (1,403)  | 2:653:B:ARG:HG2  | 2:653:B:ARG:HD2  | 20                  | 0.2      | 0.05                | 0.2        |
| (1,236)  | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 20                  | 0.18     | 0.03                | 0.18       |
| (1,236)  | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 20                  | 0.18     | 0.03                | 0.18       |
| (1,236)  | 2:709:B:GLU:HB3  | 2:709:B:GLU:HG3  | 20                  | 0.18     | 0.03                | 0.18       |
| (1,236)  | 2:625:B:GLU:HB2  | 2:625:B:GLU:HG2  | 20                  | 0.18     | 0.03                | 0.18       |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD21 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD22 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD23 | 19                  | 1.88     | 0.61                | 1.97       |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 19                  | 0.86     | 0.54                | 0.9        |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,433) | 2:716:B:LYS:HB3  | 2:708:B:ARG:HD3  | 19                  | 0.86     | 0.54                | 0.9        |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD11 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD12 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD13 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD11 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD12 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD13 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD11 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD12 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,434) | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD13 | 19                  | 0.58     | 0.64                | 0.25       |
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 19                  | 0.45     | 0.1                 | 0.49       |
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 19                  | 0.45     | 0.1                 | 0.49       |
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 19                  | 0.45     | 0.1                 | 0.49       |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 19                  | 0.39     | 0.13                | 0.39       |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 19                  | 0.39     | 0.13                | 0.39       |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 19                  | 0.39     | 0.13                | 0.39       |
| (1,158) | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG11 | 19                  | 0.39     | 0.13                | 0.39       |
| (1,158) | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG12 | 19                  | 0.39     | 0.13                | 0.39       |
| (1,158) | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG13 | 19                  | 0.39     | 0.13                | 0.39       |
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 19                  | 0.37     | 0.02                | 0.37       |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 19                  | 0.37     | 0.02                | 0.37       |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 19                  | 0.37     | 0.02                | 0.37       |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 19                  | 0.29     | 0.11                | 0.28       |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 19                  | 0.29     | 0.11                | 0.28       |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 19                  | 0.29     | 0.11                | 0.28       |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 19                  | 0.23     | 0.1                 | 0.19       |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 19                  | 0.23     | 0.1                 | 0.19       |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 19                  | 0.23     | 0.1                 | 0.19       |
| (1,274) | 2:695:B:ILE:HD11 | 2:694:B:PRO:HB2  | 19                  | 0.23     | 0.1                 | 0.19       |
| (1,274) | 2:695:B:ILE:HD12 | 2:694:B:PRO:HB2  | 19                  | 0.23     | 0.1                 | 0.19       |
| (1,274) | 2:695:B:ILE:HD13 | 2:694:B:PRO:HB2  | 19                  | 0.23     | 0.1                 | 0.19       |
| (1,209) | 2:719:B:ARG:HB3  | 2:719:B:ARG:HG2  | 19                  | 0.21     | 0.04                | 0.21       |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 19                  | 0.21     | 0.04                | 0.21       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,209)  | 2:691:B:ILE:HB   | 2:691:B:ILE:HG13 | 19                  | 0.21     | 0.04                | 0.21       |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 18                  | 1.01     | 0.13                | 0.99       |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 18                  | 1.01     | 0.13                | 0.99       |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 18                  | 1.01     | 0.13                | 0.99       |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 18                  | 0.79     | 0.68                | 0.56       |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 18                  | 0.79     | 0.68                | 0.56       |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 18                  | 0.79     | 0.68                | 0.56       |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG2  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG2  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG2  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:717:B:VAL:HG11 | 2:719:B:ARG:HG3  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:717:B:VAL:HG12 | 2:719:B:ARG:HG3  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,260)  | 2:717:B:VAL:HG13 | 2:719:B:ARG:HG3  | 18                  | 0.68     | 0.19                | 0.68       |
| (1,463)  | 2:720:B:GLU:HA   | 2:721:B:GLN:HE22 | 18                  | 0.61     | 0.4                 | 0.56       |
| (1,463)  | 2:648:B:GLU:HA   | 2:649:B:GLN:HE22 | 18                  | 0.61     | 0.4                 | 0.56       |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 18                  | 0.61     | 0.4                 | 0.56       |
| (1,488)  | 2:706:B:GLU:HA   | 2:709:B:GLU:H    | 18                  | 0.22     | 0.03                | 0.21       |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 18                  | 0.22     | 0.03                | 0.21       |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 18                  | 0.16     | 0.05                | 0.15       |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 18                  | 0.16     | 0.05                | 0.15       |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 18                  | 0.16     | 0.05                | 0.15       |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD2  | 18                  | 0.16     | 0.05                | 0.15       |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD2  | 18                  | 0.16     | 0.05                | 0.15       |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD2  | 18                  | 0.16     | 0.05                | 0.15       |
| (1,1)    | 2:614:B:GLU:HG2  | 2:614:B:GLU:HB3  | 18                  | 0.15     | 0.03                | 0.15       |
| (1,1)    | 2:616:B:GLU:HG2  | 2:616:B:GLU:HB3  | 18                  | 0.15     | 0.03                | 0.15       |
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB2  | 18                  | 0.15     | 0.03                | 0.15       |
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB3  | 18                  | 0.15     | 0.03                | 0.15       |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG21 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG22 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG23 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG21 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG22 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG23 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:697:B:LEU:HB3  | 2:631:B:ILE:HG21 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,179)  | 2:697:B:LEU:HB3  | 2:631:B:ILE:HG22 | 17                  | 0.73     | 0.32                | 0.65       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,179)  | 2:697:B:LEU:HB3  | 2:631:B:ILE:HG23 | 17                  | 0.73     | 0.32                | 0.65       |
| (1,535)  | 2:719:B:ARG:HG3  | 2:720:B:GLU:H    | 17                  | 0.56     | 0.25                | 0.56       |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 17                  | 0.56     | 0.25                | 0.56       |
| (1,535)  | 2:716:B:LYS:HD3  | 2:720:B:GLU:H    | 17                  | 0.56     | 0.25                | 0.56       |
| (1,535)  | 2:716:B:LYS:HD2  | 2:720:B:GLU:H    | 17                  | 0.56     | 0.25                | 0.56       |
| (1,1286) | 2:701:B:LYS:HD2  | 2:701:B:LYS:HG3  | 17                  | 0.2      | 0.03                | 0.21       |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 17                  | 0.2      | 0.03                | 0.21       |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 16                  | 1.48     | 0.37                | 1.62       |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 16                  | 1.48     | 0.37                | 1.62       |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 16                  | 1.48     | 0.37                | 1.62       |
| (1,213)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:HG3  | 16                  | 1.48     | 0.37                | 1.62       |
| (1,213)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:HG3  | 16                  | 1.48     | 0.37                | 1.62       |
| (1,213)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:HG3  | 16                  | 1.48     | 0.37                | 1.62       |
| (1,213)  | 2:628:B:LEU:HG   | 2:632:B:ARG:HG3  | 16                  | 1.48     | 0.37                | 1.62       |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 16                  | 0.84     | 0.37                | 1.0        |
| (1,214)  | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 16                  | 0.84     | 0.37                | 1.0        |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 16                  | 0.49     | 0.2                 | 0.44       |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 16                  | 0.49     | 0.2                 | 0.44       |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 16                  | 0.49     | 0.2                 | 0.44       |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB2  | 16                  | 0.49     | 0.2                 | 0.44       |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB2  | 16                  | 0.49     | 0.2                 | 0.44       |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB2  | 16                  | 0.49     | 0.2                 | 0.44       |
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 16                  | 0.45     | 0.08                | 0.47       |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 16                  | 0.45     | 0.08                | 0.47       |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 16                  | 0.45     | 0.08                | 0.47       |
| (1,19)   | 2:682:B:ILE:HG21 | 2:681:B:ILE:HA   | 16                  | 0.45     | 0.08                | 0.47       |
| (1,19)   | 2:682:B:ILE:HG22 | 2:681:B:ILE:HA   | 16                  | 0.45     | 0.08                | 0.47       |
| (1,19)   | 2:682:B:ILE:HG23 | 2:681:B:ILE:HA   | 16                  | 0.45     | 0.08                | 0.47       |
| (1,197)  | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 16                  | 0.42     | 0.15                | 0.4        |
| (1,197)  | 2:644:B:LEU:HD21 | 2:649:B:GLN:HA   | 16                  | 0.42     | 0.15                | 0.4        |
| (1,197)  | 2:644:B:LEU:HD22 | 2:649:B:GLN:HA   | 16                  | 0.42     | 0.15                | 0.4        |
| (1,197)  | 2:644:B:LEU:HD23 | 2:649:B:GLN:HA   | 16                  | 0.42     | 0.15                | 0.4        |
| (1,197)  | 2:641:B:LEU:HD11 | 2:649:B:GLN:HA   | 16                  | 0.42     | 0.15                | 0.4        |
| (1,197)  | 2:641:B:LEU:HD12 | 2:649:B:GLN:HA   | 16                  | 0.42     | 0.15                | 0.4        |
| (1,197)  | 2:641:B:LEU:HD13 | 2:649:B:GLN:HA   | 16                  | 0.42     | 0.15                | 0.4        |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 16                  | 0.41     | 0.13                | 0.42       |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 16                  | 0.41     | 0.13                | 0.42       |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 16                  | 0.41     | 0.13                | 0.42       |
| (1,688)  | 2:670:B:LEU:HD11 | 2:685:B:LEU:H    | 16                  | 0.41     | 0.13                | 0.42       |
| (1,688)  | 2:670:B:LEU:HD12 | 2:685:B:LEU:H    | 16                  | 0.41     | 0.13                | 0.42       |
| (1,688)  | 2:670:B:LEU:HD13 | 2:685:B:LEU:H    | 16                  | 0.41     | 0.13                | 0.42       |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 15                  | 0.75     | 0.2                 | 0.8        |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,279) | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,279) | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,279) | 2:697:B:LEU:HD11 | 2:638:B:GLN:HG3  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,279) | 2:697:B:LEU:HD12 | 2:638:B:GLN:HG3  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,279) | 2:697:B:LEU:HD13 | 2:638:B:GLN:HG3  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,279) | 2:620:B:LEU:HD11 | 2:711:B:GLN:HG2  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,279) | 2:620:B:LEU:HD12 | 2:711:B:GLN:HG2  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,279) | 2:620:B:LEU:HD13 | 2:711:B:GLN:HG2  | 15                  | 0.75     | 0.2                 | 0.8        |
| (1,251) | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB1  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB2  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB3  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB1  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB2  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB3  | 15                  | 0.46     | 0.1                 | 0.47       |
| (1,499) | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 15                  | 0.35     | 0.12                | 0.37       |
| (1,499) | 2:620:B:LEU:HB2  | 2:622:B:VAL:H    | 15                  | 0.35     | 0.12                | 0.37       |
| (1,364) | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 15                  | 0.2      | 0.05                | 0.21       |
| (1,364) | 2:640:B:LYS:HB3  | 2:640:B:LYS:HA   | 15                  | 0.2      | 0.05                | 0.21       |
| (1,364) | 2:686:B:ARG:HB3  | 2:686:B:ARG:HA   | 15                  | 0.2      | 0.05                | 0.21       |
| (1,364) | 2:639:B:LYS:HB2  | 2:639:B:LYS:HA   | 15                  | 0.2      | 0.05                | 0.21       |
| (1,364) | 2:640:B:LYS:HB2  | 2:640:B:LYS:HA   | 15                  | 0.2      | 0.05                | 0.21       |
| (1,364) | 2:706:B:GLU:HB2  | 2:706:B:GLU:HA   | 15                  | 0.2      | 0.05                | 0.21       |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD21 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD22 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD23 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD21 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD22 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD23 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD21 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD22 | 14                  | 0.34     | 0.16                | 0.32       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,188)  | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD23 | 14                  | 0.34     | 0.16                | 0.32       |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 14                  | 0.27     | 0.11                | 0.21       |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 14                  | 0.27     | 0.11                | 0.21       |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 14                  | 0.27     | 0.11                | 0.21       |
| (1,138)  | 2:637:B:ILE:HB   | 2:657:B:THR:HG21 | 14                  | 0.27     | 0.11                | 0.21       |
| (1,138)  | 2:637:B:ILE:HB   | 2:657:B:THR:HG22 | 14                  | 0.27     | 0.11                | 0.21       |
| (1,138)  | 2:637:B:ILE:HB   | 2:657:B:THR:HG23 | 14                  | 0.27     | 0.11                | 0.21       |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 14                  | 0.24     | 0.09                | 0.24       |
| (1,1921) | 2:724:B:LYS:HG3  | 2:725:B:TYR:H    | 14                  | 0.24     | 0.09                | 0.24       |
| (1,511)  | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 14                  | 0.18     | 0.02                | 0.19       |
| (1,211)  | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG3  | 14                  | 0.14     | 0.02                | 0.14       |
| (1,211)  | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG2  | 14                  | 0.14     | 0.02                | 0.14       |
| (1,211)  | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 14                  | 0.14     | 0.02                | 0.14       |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 13                  | 0.67     | 0.51                | 0.65       |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 13                  | 0.61     | 0.2                 | 0.67       |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 13                  | 0.61     | 0.2                 | 0.67       |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 13                  | 0.61     | 0.2                 | 0.67       |
| (1,441)  | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG21 | 13                  | 0.61     | 0.2                 | 0.67       |
| (1,441)  | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG22 | 13                  | 0.61     | 0.2                 | 0.67       |
| (1,441)  | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG23 | 13                  | 0.61     | 0.2                 | 0.67       |
| (1,1852) | 2:701:B:LYS:HD2  | 2:700:B:LEU:H    | 13                  | 0.51     | 0.16                | 0.52       |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 13                  | 0.51     | 0.16                | 0.52       |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD21 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD22 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD23 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:652:B:PHE:HB2  | 2:644:B:LEU:HD21 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:652:B:PHE:HB2  | 2:644:B:LEU:HD22 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,51)   | 2:652:B:PHE:HB2  | 2:644:B:LEU:HD23 | 13                  | 0.46     | 0.32                | 0.32       |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 13                  | 0.3      | 0.13                | 0.3        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD11 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD12 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD13 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD11 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD12 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD13 | 13                  | 0.3      | 0.13                | 0.3        |
| (1,85)   | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 13                  | 0.26     | 0.08                | 0.27       |
| (1,85)   | 2:625:B:GLU:HA   | 2:625:B:GLU:HG2  | 13                  | 0.26     | 0.08                | 0.27       |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 12                  | 1.16     | 0.25                | 1.18       |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 12                  | 1.16     | 0.25                | 1.18       |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 12                  | 1.16     | 0.25                | 1.18       |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 12                  | 0.87     | 0.56                | 1.14       |
| (1,429)  | 2:717:B:VAL:HA   | 2:716:B:LYS:HD2  | 12                  | 0.58     | 0.14                | 0.62       |
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD2  | 12                  | 0.58     | 0.14                | 0.62       |
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD3  | 12                  | 0.58     | 0.14                | 0.62       |
| (1,429)  | 2:640:B:LYS:HA   | 2:640:B:LYS:HD3  | 12                  | 0.58     | 0.14                | 0.62       |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD11 | 2:657:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD11 | 2:657:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD11 | 2:657:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD12 | 2:657:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD12 | 2:657:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD12 | 2:657:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD13 | 2:657:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD13 | 2:657:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD13 | 2:657:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD21 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD21 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD21 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD22 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD22 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,256)  | 2:658:B:LEU:HD22 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD23 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD23 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD23 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD11 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD11 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD11 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD12 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD12 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD12 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD13 | 2:630:B:THR:HG21 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD13 | 2:630:B:THR:HG22 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,256)  | 2:658:B:LEU:HD13 | 2:630:B:THR:HG23 | 12                  | 0.53     | 0.18                | 0.54       |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD3  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD3  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD3  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD2  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD2  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD2  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD11 | 2:686:B:ARG:HD2  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD12 | 2:686:B:ARG:HD2  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD13 | 2:686:B:ARG:HD2  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD21 | 2:667:B:ARG:HD3  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD22 | 2:667:B:ARG:HD3  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,14)   | 2:658:B:LEU:HD23 | 2:667:B:ARG:HD3  | 12                  | 0.47     | 0.2                 | 0.42       |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 12                  | 0.37     | 0.19                | 0.43       |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 12                  | 0.37     | 0.19                | 0.43       |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 12                  | 0.37     | 0.19                | 0.43       |
| (1,514)  | 2:700:B:LEU:HG   | 2:699:B:ARG:H    | 12                  | 0.37     | 0.19                | 0.43       |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2  | 12                  | 0.19     | 0.07                | 0.15       |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2  | 12                  | 0.19     | 0.07                | 0.15       |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2  | 12                  | 0.19     | 0.07                | 0.15       |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE3  | 12                  | 0.19     | 0.07                | 0.15       |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE3  | 12                  | 0.19     | 0.07                | 0.15       |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE3  | 12                  | 0.19     | 0.07                | 0.15       |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 12                  | 0.15     | 0.02                | 0.14       |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 12                  | 0.15     | 0.02                | 0.14       |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 12                  | 0.15     | 0.02                | 0.14       |
| (1,391)  | 2:728:B:LYS:HB3  | 2:728:B:LYS:HE2  | 11                  | 0.76     | 0.11                | 0.81       |
| (1,391)  | 2:728:B:LYS:HB3  | 2:728:B:LYS:HE3  | 11                  | 0.76     | 0.11                | 0.81       |
| (1,391)  | 2:716:B:LYS:HB2  | 2:716:B:LYS:HE2  | 11                  | 0.76     | 0.11                | 0.81       |
| (1,391)  | 2:716:B:LYS:HB3  | 2:716:B:LYS:HE2  | 11                  | 0.76     | 0.11                | 0.81       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,391)  | 2:716:B:LYS:HB3  | 2:716:B:LYS:HE3  | 11                  | 0.76     | 0.11                | 0.81       |
| (1,432)  | 2:720:B:GLU:HB3  | 2:724:B:LYS:HE2  | 11                  | 0.59     | 0.28                | 0.6        |
| (1,432)  | 2:634:B:LEU:HB3  | 2:701:B:LYS:HE3  | 11                  | 0.59     | 0.28                | 0.6        |
| (1,432)  | 2:664:B:VAL:HB   | 2:668:B:LYS:HE2  | 11                  | 0.59     | 0.28                | 0.6        |
| (1,432)  | 2:700:B:LEU:HG   | 2:701:B:LYS:HE2  | 11                  | 0.59     | 0.28                | 0.6        |
| (1,432)  | 2:700:B:LEU:HG   | 2:701:B:LYS:HE3  | 11                  | 0.59     | 0.28                | 0.6        |
| (1,432)  | 2:664:B:VAL:HB   | 2:668:B:LYS:HE3  | 11                  | 0.59     | 0.28                | 0.6        |
| (1,432)  | 2:720:B:GLU:HB3  | 2:724:B:LYS:HE3  | 11                  | 0.59     | 0.28                | 0.6        |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 11                  | 0.45     | 0.22                | 0.43       |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD3  | 11                  | 0.41     | 0.15                | 0.38       |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD2  | 11                  | 0.41     | 0.15                | 0.38       |
| (1,66)   | 2:636:B:ALA:HA   | 2:639:B:LYS:HD3  | 11                  | 0.41     | 0.15                | 0.38       |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD21 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD22 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD23 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:649:B:GLN:HA   | 2:641:B:LEU:HD11 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:649:B:GLN:HA   | 2:641:B:LEU:HD12 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,49)   | 2:649:B:GLN:HA   | 2:641:B:LEU:HD13 | 11                  | 0.4      | 0.23                | 0.38       |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 11                  | 0.37     | 0.06                | 0.38       |
| (1,1548) | 2:672:B:ARG:HD3  | 2:672:B:ARG:HA   | 11                  | 0.37     | 0.06                | 0.38       |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 11                  | 0.23     | 0.05                | 0.24       |
| (1,1276) | 2:654:B:LEU:HD21 | 2:686:B:ARG:HA   | 11                  | 0.22     | 0.09                | 0.19       |
| (1,1276) | 2:654:B:LEU:HD22 | 2:686:B:ARG:HA   | 11                  | 0.22     | 0.09                | 0.19       |
| (1,1276) | 2:654:B:LEU:HD23 | 2:686:B:ARG:HA   | 11                  | 0.22     | 0.09                | 0.19       |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 11                  | 0.22     | 0.09                | 0.19       |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 11                  | 0.22     | 0.09                | 0.19       |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 11                  | 0.22     | 0.09                | 0.19       |
| (1,562)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 11                  | 0.16     | 0.03                | 0.16       |
| (1,562)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 11                  | 0.16     | 0.03                | 0.16       |
| (1,562)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 11                  | 0.16     | 0.03                | 0.16       |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 11                  | 0.14     | 0.01                | 0.14       |
| (1,758)  | 1:206:A:GLN:HG3  | 1:206:A:GLN:HB3  | 11                  | 0.13     | 0.02                | 0.12       |
| (1,758)  | 1:214:A:GLU:HG2  | 1:214:A:GLU:HB3  | 11                  | 0.13     | 0.02                | 0.12       |
| (1,758)  | 1:206:A:GLN:HG2  | 1:206:A:GLN:HB3  | 11                  | 0.13     | 0.02                | 0.12       |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 10                  | 1.37     | 0.36                | 1.28       |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 10                  | 1.37     | 0.36                | 1.28       |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 10                  | 1.37     | 0.36                | 1.28       |
| (1,440)  | 2:697:B:LEU:HD21 | 2:638:B:GLN:HG3  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,440)  | 2:697:B:LEU:HD22 | 2:638:B:GLN:HG3  | 10                  | 0.96     | 0.28                | 1.06       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,440) | 2:697:B:LEU:HD23 | 2:638:B:GLN:HG3  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,440) | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,440) | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,440) | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,440) | 2:620:B:LEU:HD21 | 2:711:B:GLN:HG2  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,440) | 2:620:B:LEU:HD22 | 2:711:B:GLN:HG2  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,440) | 2:620:B:LEU:HD23 | 2:711:B:GLN:HG2  | 10                  | 0.96     | 0.28                | 1.06       |
| (1,952) | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 10                  | 0.82     | 0.27                | 0.8        |
| (1,952) | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 10                  | 0.82     | 0.27                | 0.8        |
| (1,952) | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 10                  | 0.82     | 0.27                | 0.8        |
| (1,456) | 1:226:A:LEU:HB3  | 2:688:B:ASN:HD21 | 10                  | 0.78     | 0.19                | 0.74       |
| (1,456) | 2:687:B:LYS:HD2  | 2:688:B:ASN:HD21 | 10                  | 0.78     | 0.19                | 0.74       |
| (1,456) | 2:687:B:LYS:HD3  | 2:688:B:ASN:HD21 | 10                  | 0.78     | 0.19                | 0.74       |
| (1,456) | 1:223:A:LEU:HB3  | 2:688:B:ASN:HD21 | 10                  | 0.78     | 0.19                | 0.74       |
| (1,15)  | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:654:B:LEU:HD21 | 2:686:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:654:B:LEU:HD22 | 2:686:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:654:B:LEU:HD23 | 2:686:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD2  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD2  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD2  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:631:B:ILE:HG21 | 2:632:B:ARG:HD2  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:631:B:ILE:HG22 | 2:632:B:ARG:HD2  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:631:B:ILE:HG23 | 2:632:B:ARG:HD2  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:664:B:VAL:HG21 | 2:667:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:664:B:VAL:HG22 | 2:667:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,15)  | 2:664:B:VAL:HG23 | 2:667:B:ARG:HD3  | 10                  | 0.69     | 0.38                | 0.59       |
| (1,16)  | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD2  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD2  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD2  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:624:B:LEU:HD21 | 2:708:B:ARG:HD2  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:624:B:LEU:HD22 | 2:708:B:ARG:HD2  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:624:B:LEU:HD23 | 2:708:B:ARG:HD2  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD3  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD3  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD3  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:664:B:VAL:HG21 | 2:667:B:ARG:HD3  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:664:B:VAL:HG22 | 2:667:B:ARG:HD3  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,16)  | 2:664:B:VAL:HG23 | 2:667:B:ARG:HD3  | 10                  | 0.67     | 0.42                | 0.57       |
| (1,761) | 2:711:B:GLN:HA   | 1:207:A:LEU:HD21 | 10                  | 0.63     | 0.32                | 0.74       |

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| Key     | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,761) | 2:711:B:GLN:HA  | 1:207:A:LEU:HD22 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,761) | 2:711:B:GLN:HA  | 1:207:A:LEU:HD23 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,761) | 2:713:B:GLY:HA3 | 1:207:A:LEU:HD21 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,761) | 2:713:B:GLY:HA3 | 1:207:A:LEU:HD22 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,761) | 2:713:B:GLY:HA3 | 1:207:A:LEU:HD23 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,761) | 2:620:B:LEU:HA  | 1:207:A:LEU:HD21 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,761) | 2:620:B:LEU:HA  | 1:207:A:LEU:HD22 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,761) | 2:620:B:LEU:HA  | 1:207:A:LEU:HD23 | 10                  | 0.63     | 0.32                | 0.74       |
| (1,159) | 2:697:B:LEU:HG  | 2:693:B:VAL:HG11 | 10                  | 0.45     | 0.44                | 0.32       |
| (1,159) | 2:697:B:LEU:HG  | 2:693:B:VAL:HG12 | 10                  | 0.45     | 0.44                | 0.32       |
| (1,159) | 2:697:B:LEU:HG  | 2:693:B:VAL:HG13 | 10                  | 0.45     | 0.44                | 0.32       |
| (1,12)  | 2:611:B:TYR:HD1 | 2:614:B:GLU:HA   | 10                  | 0.41     | 0.24                | 0.36       |
| (1,12)  | 2:611:B:TYR:HD2 | 2:614:B:GLU:HA   | 10                  | 0.41     | 0.24                | 0.36       |
| (1,12)  | 2:718:B:TRP:HZ3 | 2:723:B:GLU:HA   | 10                  | 0.41     | 0.24                | 0.36       |
| (1,12)  | 2:611:B:TYR:HD1 | 2:616:B:GLU:HA   | 10                  | 0.41     | 0.24                | 0.36       |
| (1,12)  | 2:611:B:TYR:HD2 | 2:616:B:GLU:HA   | 10                  | 0.41     | 0.24                | 0.36       |
| (1,133) | 2:649:B:GLN:HG2 | 2:644:B:LEU:HD11 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:649:B:GLN:HG2 | 2:644:B:LEU:HD12 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:649:B:GLN:HG2 | 2:644:B:LEU:HD13 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:638:B:GLN:HG3 | 2:693:B:VAL:HG21 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:638:B:GLN:HG3 | 2:693:B:VAL:HG22 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:638:B:GLN:HG3 | 2:693:B:VAL:HG23 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:648:B:GLU:HG2 | 2:644:B:LEU:HD11 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:648:B:GLU:HG2 | 2:644:B:LEU:HD12 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,133) | 2:648:B:GLU:HG2 | 2:644:B:LEU:HD13 | 10                  | 0.38     | 0.13                | 0.38       |
| (1,182) | 2:678:B:ALA:HB1 | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB1 | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB1 | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB2 | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB2 | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB2 | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB3 | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB3 | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:678:B:ALA:HB3 | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB1 | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB1 | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB1 | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB2 | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB2 | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB2 | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB3 | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182) | 2:679:B:ALA:HB3 | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,182)  | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG21 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG22 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG23 | 10                  | 0.36     | 0.15                | 0.38       |
| (1,235)  | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 10                  | 0.32     | 0.12                | 0.35       |
| (1,235)  | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 10                  | 0.32     | 0.12                | 0.35       |
| (1,235)  | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 10                  | 0.32     | 0.12                | 0.35       |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD21 | 10                  | 0.27     | 0.08                | 0.29       |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD22 | 10                  | 0.27     | 0.08                | 0.29       |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD23 | 10                  | 0.27     | 0.08                | 0.29       |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD21 | 10                  | 0.27     | 0.08                | 0.29       |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD22 | 10                  | 0.27     | 0.08                | 0.29       |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD23 | 10                  | 0.27     | 0.08                | 0.29       |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 10                  | 0.25     | 0.1                 | 0.25       |
| (1,614)  | 2:640:B:LYS:HB3  | 2:642:B:SER:H    | 10                  | 0.25     | 0.1                 | 0.25       |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 10                  | 0.17     | 0.05                | 0.16       |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD11 | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD12 | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD13 | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 9                   | 1.08     | 0.76                | 0.67       |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 9                   | 1.08     | 0.76                | 0.67       |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 9                   | 1.08     | 0.76                | 0.67       |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD11 | 9                   | 1.08     | 0.76                | 0.67       |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD12 | 9                   | 1.08     | 0.76                | 0.67       |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD13 | 9                   | 1.08     | 0.76                | 0.67       |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 9                   | 0.96     | 0.25                | 1.02       |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 9                   | 0.96     | 0.25                | 1.02       |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 9                   | 0.96     | 0.25                | 1.02       |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD3  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD3  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD3  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD2  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD2  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD2  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD21 | 2:640:B:LYS:HD3  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD22 | 2:640:B:LYS:HD3  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,271)  | 2:644:B:LEU:HD23 | 2:640:B:LYS:HD3  | 9                   | 0.86     | 0.25                | 0.86       |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 9                   | 0.77     | 0.02                | 0.78       |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 9                   | 0.77     | 0.02                | 0.78       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 9                   | 0.77     | 0.02                | 0.78       |
| (1,74)   | 2:613:B:CYS:HB3  | 2:612:B:ARG:HB2  | 9                   | 0.66     | 0.33                | 0.89       |
| (1,74)   | 2:613:B:CYS:HB2  | 2:612:B:ARG:HB2  | 9                   | 0.66     | 0.33                | 0.89       |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 9                   | 0.66     | 0.22                | 0.77       |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 9                   | 0.58     | 0.38                | 0.4        |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 9                   | 0.58     | 0.38                | 0.4        |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 9                   | 0.58     | 0.38                | 0.4        |
| (1,129)  | 2:632:B:ARG:HG2  | 2:633:B:VAL:HG21 | 9                   | 0.58     | 0.38                | 0.4        |
| (1,129)  | 2:632:B:ARG:HG2  | 2:633:B:VAL:HG22 | 9                   | 0.58     | 0.38                | 0.4        |
| (1,129)  | 2:632:B:ARG:HG2  | 2:633:B:VAL:HG23 | 9                   | 0.58     | 0.38                | 0.4        |
| (1,266)  | 2:658:B:LEU:HD11 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:658:B:LEU:HD12 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:658:B:LEU:HD13 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:631:B:ILE:HD11 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:631:B:ILE:HD12 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:631:B:ILE:HD13 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:685:B:LEU:HD21 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:685:B:LEU:HD22 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,266)  | 2:685:B:LEU:HD23 | 2:634:B:LEU:HG   | 9                   | 0.46     | 0.24                | 0.47       |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 9                   | 0.36     | 0.16                | 0.37       |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 9                   | 0.36     | 0.16                | 0.37       |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 9                   | 0.36     | 0.16                | 0.37       |
| (1,384)  | 2:697:B:LEU:HD11 | 2:694:B:PRO:HA   | 9                   | 0.33     | 0.09                | 0.31       |
| (1,384)  | 2:697:B:LEU:HD12 | 2:694:B:PRO:HA   | 9                   | 0.33     | 0.09                | 0.31       |
| (1,384)  | 2:697:B:LEU:HD13 | 2:694:B:PRO:HA   | 9                   | 0.33     | 0.09                | 0.31       |
| (1,384)  | 2:693:B:VAL:HG21 | 2:694:B:PRO:HA   | 9                   | 0.33     | 0.09                | 0.31       |
| (1,384)  | 2:693:B:VAL:HG22 | 2:694:B:PRO:HA   | 9                   | 0.33     | 0.09                | 0.31       |
| (1,384)  | 2:693:B:VAL:HG23 | 2:694:B:PRO:HA   | 9                   | 0.33     | 0.09                | 0.31       |
| (1,267)  | 2:637:B:ILE:HD11 | 2:640:B:LYS:HD3  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:637:B:ILE:HD12 | 2:640:B:LYS:HD3  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:637:B:ILE:HD13 | 2:640:B:LYS:HD3  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD3  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD3  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD3  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:637:B:ILE:HD11 | 2:640:B:LYS:HD2  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:637:B:ILE:HD12 | 2:640:B:LYS:HD2  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:637:B:ILE:HD13 | 2:640:B:LYS:HD2  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD2  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD2  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,267)  | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD2  | 9                   | 0.31     | 0.2                 | 0.22       |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 9                   | 0.31     | 0.02                | 0.32       |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 9                   | 0.31     | 0.02                | 0.32       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 9                   | 0.31     | 0.02                | 0.32       |
| (1,147)  | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 9                   | 0.3      | 0.0                 | 0.3        |
| (1,147)  | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 9                   | 0.3      | 0.0                 | 0.3        |
| (1,147)  | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 9                   | 0.3      | 0.0                 | 0.3        |
| (1,589)  | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 9                   | 0.19     | 0.09                | 0.17       |
| (1,589)  | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 9                   | 0.19     | 0.09                | 0.17       |
| (1,589)  | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 9                   | 0.19     | 0.09                | 0.17       |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD21 | 9                   | 0.16     | 0.06                | 0.12       |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD22 | 9                   | 0.16     | 0.06                | 0.12       |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD23 | 9                   | 0.16     | 0.06                | 0.12       |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD21 | 9                   | 0.16     | 0.06                | 0.12       |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD22 | 9                   | 0.16     | 0.06                | 0.12       |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD23 | 9                   | 0.16     | 0.06                | 0.12       |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 9                   | 0.15     | 0.04                | 0.15       |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H    | 9                   | 0.13     | 0.02                | 0.13       |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 8                   | 1.68     | 0.2                 | 1.71       |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 8                   | 1.68     | 0.2                 | 1.71       |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 8                   | 1.68     | 0.2                 | 1.71       |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 8                   | 0.8      | 0.08                | 0.8        |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 8                   | 0.8      | 0.08                | 0.8        |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 8                   | 0.8      | 0.08                | 0.8        |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 8                   | 0.75     | 0.41                | 0.64       |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 8                   | 0.75     | 0.41                | 0.64       |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 8                   | 0.75     | 0.41                | 0.64       |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD11 | 8                   | 0.74     | 0.47                | 0.64       |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD12 | 8                   | 0.74     | 0.47                | 0.64       |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD13 | 8                   | 0.74     | 0.47                | 0.64       |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD11 | 8                   | 0.74     | 0.47                | 0.64       |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD12 | 8                   | 0.74     | 0.47                | 0.64       |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD13 | 8                   | 0.74     | 0.47                | 0.64       |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 8                   | 0.45     | 0.28                | 0.34       |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 8                   | 0.45     | 0.28                | 0.34       |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 8                   | 0.45     | 0.28                | 0.34       |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG3  | 8                   | 0.39     | 0.04                | 0.39       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG2  | 8                   | 0.39     | 0.04                | 0.39       |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 8                   | 0.34     | 0.11                | 0.37       |
| (1,2458) | 2:703:B:LYS:HG2  | 2:707:B:TRP:HE1  | 8                   | 0.34     | 0.11                | 0.37       |
| (1,1354) | 2:716:B:LYS:HD3  | 2:720:B:GLU:HG3  | 8                   | 0.32     | 0.11                | 0.31       |
| (1,1354) | 2:716:B:LYS:HD2  | 2:720:B:GLU:HG3  | 8                   | 0.32     | 0.11                | 0.31       |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 8                   | 0.24     | 0.05                | 0.24       |
| (1,754)  | 2:673:B:ILE:HG21 | 2:707:B:TRP:HE1  | 8                   | 0.24     | 0.07                | 0.24       |
| (1,754)  | 2:673:B:ILE:HG22 | 2:707:B:TRP:HE1  | 8                   | 0.24     | 0.07                | 0.24       |
| (1,754)  | 2:673:B:ILE:HG23 | 2:707:B:TRP:HE1  | 8                   | 0.24     | 0.07                | 0.24       |
| (1,754)  | 2:703:B:LYS:HB3  | 2:707:B:TRP:HE1  | 8                   | 0.24     | 0.07                | 0.24       |
| (1,204)  | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD11 | 8                   | 0.23     | 0.1                 | 0.25       |
| (1,204)  | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD12 | 8                   | 0.23     | 0.1                 | 0.25       |
| (1,204)  | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD13 | 8                   | 0.23     | 0.1                 | 0.25       |
| (1,204)  | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD11 | 8                   | 0.23     | 0.1                 | 0.25       |
| (1,204)  | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD12 | 8                   | 0.23     | 0.1                 | 0.25       |
| (1,204)  | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD13 | 8                   | 0.23     | 0.1                 | 0.25       |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 8                   | 0.21     | 0.02                | 0.22       |
| (1,396)  | 2:686:B:ARG:HB2  | 2:686:B:ARG:HD3  | 8                   | 0.2      | 0.15                | 0.15       |
| (1,396)  | 2:632:B:ARG:HB2  | 2:632:B:ARG:HD2  | 8                   | 0.2      | 0.15                | 0.15       |
| (1,396)  | 2:632:B:ARG:HG3  | 2:632:B:ARG:HD2  | 8                   | 0.2      | 0.15                | 0.15       |
| (1,396)  | 2:667:B:ARG:HB2  | 2:667:B:ARG:HD3  | 8                   | 0.2      | 0.15                | 0.15       |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 7                   | 1.6      | 0.25                | 1.58       |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 7                   | 1.6      | 0.25                | 1.58       |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 7                   | 1.6      | 0.25                | 1.58       |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 7                   | 1.6      | 0.25                | 1.58       |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 7                   | 1.6      | 0.25                | 1.58       |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 7                   | 1.6      | 0.25                | 1.58       |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 7                   | 1.53     | 0.22                | 1.53       |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 7                   | 1.53     | 0.22                | 1.53       |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 7                   | 1.53     | 0.22                | 1.53       |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 7                   | 1.53     | 0.22                | 1.53       |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 7                   | 1.53     | 0.22                | 1.53       |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 7                   | 1.53     | 0.22                | 1.53       |
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 7                   | 1.48     | 0.87                | 1.3        |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 7                   | 1.48     | 0.87                | 1.3        |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 7                   | 1.48     | 0.87                | 1.3        |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 7                   | 0.93     | 0.61                | 0.76       |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 7                   | 0.93     | 0.61                | 0.76       |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 7                   | 0.93     | 0.61                | 0.76       |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 7                   | 0.93     | 0.61                | 0.76       |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 7                   | 0.93     | 0.61                | 0.76       |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 7                   | 0.93     | 0.61                | 0.76       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 7                   | 0.93     | 0.61                | 0.76       |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 7                   | 0.93     | 0.61                | 0.76       |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 7                   | 0.93     | 0.61                | 0.76       |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 7                   | 0.76     | 0.42                | 0.62       |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 7                   | 0.75     | 0.02                | 0.75       |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 7                   | 0.75     | 0.02                | 0.75       |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 7                   | 0.75     | 0.02                | 0.75       |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 7                   | 0.74     | 0.49                | 0.6        |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 7                   | 0.54     | 0.34                | 0.5        |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 7                   | 0.54     | 0.34                | 0.5        |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 7                   | 0.54     | 0.34                | 0.5        |
| (1,394)  | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE3  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE3  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE3  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE2  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE2  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE2  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:717:B:VAL:HG21 | 2:716:B:LYS:HE3  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:717:B:VAL:HG22 | 2:716:B:LYS:HE3  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,394)  | 2:717:B:VAL:HG23 | 2:716:B:LYS:HE3  | 7                   | 0.53     | 0.31                | 0.66       |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE3  | 7                   | 0.52     | 0.64                | 0.37       |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE3  | 7                   | 0.52     | 0.64                | 0.37       |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE3  | 7                   | 0.52     | 0.64                | 0.37       |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE2  | 7                   | 0.52     | 0.64                | 0.37       |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE2  | 7                   | 0.52     | 0.64                | 0.37       |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE2  | 7                   | 0.52     | 0.64                | 0.37       |
| (1,574)  | 2:665:B:ILE:HD11 | 2:630:B:THR:H    | 7                   | 0.5      | 0.14                | 0.56       |
| (1,574)  | 2:665:B:ILE:HD12 | 2:630:B:THR:H    | 7                   | 0.5      | 0.14                | 0.56       |
| (1,574)  | 2:665:B:ILE:HD13 | 2:630:B:THR:H    | 7                   | 0.5      | 0.14                | 0.56       |
| (1,574)  | 2:631:B:ILE:HG21 | 2:630:B:THR:H    | 7                   | 0.5      | 0.14                | 0.56       |
| (1,574)  | 2:631:B:ILE:HG22 | 2:630:B:THR:H    | 7                   | 0.5      | 0.14                | 0.56       |
| (1,574)  | 2:631:B:ILE:HG23 | 2:630:B:THR:H    | 7                   | 0.5      | 0.14                | 0.56       |
| (1,359)  | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 7                   | 0.45     | 0.14                | 0.52       |
| (1,278)  | 2:670:B:LEU:HD21 | 2:696:B:VAL:HB   | 7                   | 0.41     | 0.07                | 0.42       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,278)  | 2:670:B:LEU:HD22 | 2:696:B:VAL:HB   | 7                   | 0.41     | 0.07                | 0.42       |
| (1,278)  | 2:670:B:LEU:HD23 | 2:696:B:VAL:HB   | 7                   | 0.41     | 0.07                | 0.42       |
| (1,278)  | 2:685:B:LEU:HD11 | 2:696:B:VAL:HB   | 7                   | 0.41     | 0.07                | 0.42       |
| (1,278)  | 2:685:B:LEU:HD12 | 2:696:B:VAL:HB   | 7                   | 0.41     | 0.07                | 0.42       |
| (1,278)  | 2:685:B:LEU:HD13 | 2:696:B:VAL:HB   | 7                   | 0.41     | 0.07                | 0.42       |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 7                   | 0.4      | 0.07                | 0.4        |
| (1,2197) | 2:677:B:LYS:HE2  | 2:677:B:LYS:H    | 7                   | 0.39     | 0.24                | 0.33       |
| (1,2197) | 2:677:B:LYS:HE3  | 2:677:B:LYS:H    | 7                   | 0.39     | 0.24                | 0.33       |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 7                   | 0.39     | 0.02                | 0.38       |
| (1,415)  | 2:703:B:LYS:HB3  | 2:702:B:MET:HE1  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:703:B:LYS:HB3  | 2:702:B:MET:HE2  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:703:B:LYS:HB3  | 2:702:B:MET:HE3  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE1  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE2  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE3  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE1  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE2  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE3  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE1  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE2  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE3  | 7                   | 0.38     | 0.18                | 0.35       |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 7                   | 0.37     | 0.04                | 0.38       |
| (1,619)  | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 7                   | 0.35     | 0.17                | 0.33       |
| (1,126)  | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG21 | 7                   | 0.31     | 0.1                 | 0.32       |
| (1,126)  | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG22 | 7                   | 0.31     | 0.1                 | 0.32       |
| (1,126)  | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG23 | 7                   | 0.31     | 0.1                 | 0.32       |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG21 | 7                   | 0.31     | 0.1                 | 0.32       |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG22 | 7                   | 0.31     | 0.1                 | 0.32       |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG23 | 7                   | 0.31     | 0.1                 | 0.32       |
| (1,63)   | 2:630:B:THR:HA   | 2:634:B:LEU:HG   | 7                   | 0.28     | 0.16                | 0.22       |
| (1,63)   | 2:630:B:THR:HA   | 2:632:B:ARG:HG3  | 7                   | 0.28     | 0.16                | 0.22       |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 7                   | 0.27     | 0.14                | 0.25       |
| (1,354)  | 2:715:B:ASN:HB2  | 2:712:B:ARG:HA   | 7                   | 0.24     | 0.09                | 0.21       |
| (1,354)  | 2:674:B:TYR:HB3  | 2:671:B:GLN:HA   | 7                   | 0.24     | 0.09                | 0.21       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,354)  | 2:715:B:ASN:HB3  | 2:712:B:ARG:HA   | 7                   | 0.24     | 0.09                | 0.21       |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 7                   | 0.22     | 0.03                | 0.23       |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 7                   | 0.17     | 0.02                | 0.17       |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 7                   | 0.17     | 0.02                | 0.17       |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 7                   | 0.17     | 0.02                | 0.17       |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 7                   | 0.13     | 0.02                | 0.12       |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 7                   | 0.13     | 0.02                | 0.12       |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 7                   | 0.13     | 0.02                | 0.12       |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB2  | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB3  | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1719) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE22 | 6                   | 1.36     | 0.7                 | 1.46       |
| (1,1719) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE22 | 6                   | 1.36     | 0.7                 | 1.46       |
| (1,1719) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE22 | 6                   | 1.36     | 0.7                 | 1.46       |
| (1,2304) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE21 | 6                   | 1.15     | 0.5                 | 1.23       |
| (1,2304) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE21 | 6                   | 1.15     | 0.5                 | 1.23       |
| (1,2304) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE21 | 6                   | 1.15     | 0.5                 | 1.23       |
| (1,854)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD2  | 6                   | 0.82     | 0.01                | 0.82       |
| (1,854)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD2  | 6                   | 0.82     | 0.01                | 0.82       |
| (1,854)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD2  | 6                   | 0.82     | 0.01                | 0.82       |
| (1,1489) | 2:653:B:ARG:HD2  | 2:687:B:LYS:HA   | 6                   | 0.81     | 0.38                | 0.78       |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,192)  | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD11 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD12 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,192)  | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD13 | 6                   | 0.66     | 0.34                | 0.63       |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG11 | 6                   | 0.49     | 0.27                | 0.58       |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG12 | 6                   | 0.49     | 0.27                | 0.58       |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG13 | 6                   | 0.49     | 0.27                | 0.58       |
| (1,131)  | 2:672:B:ARG:HD2  | 2:623:B:VAL:HG11 | 6                   | 0.49     | 0.27                | 0.58       |
| (1,131)  | 2:672:B:ARG:HD2  | 2:623:B:VAL:HG12 | 6                   | 0.49     | 0.27                | 0.58       |
| (1,131)  | 2:672:B:ARG:HD2  | 2:623:B:VAL:HG13 | 6                   | 0.49     | 0.27                | 0.58       |
| (1,1682) | 2:606:B:ASN:HB2  | 2:610:B:ILE:HG13 | 6                   | 0.49     | 0.24                | 0.46       |
| (1,389)  | 2:677:B:LYS:HG2  | 2:677:B:LYS:HE2  | 6                   | 0.47     | 0.23                | 0.5        |
| (1,389)  | 2:687:B:LYS:HG3  | 2:687:B:LYS:HE3  | 6                   | 0.47     | 0.23                | 0.5        |
| (1,389)  | 2:677:B:LYS:HG2  | 2:677:B:LYS:HE3  | 6                   | 0.47     | 0.23                | 0.5        |
| (1,2413) | 2:699:B:ARG:HG3  | 2:699:B:ARG:H    | 6                   | 0.41     | 0.08                | 0.44       |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD21 | 6                   | 0.37     | 0.14                | 0.42       |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD22 | 6                   | 0.37     | 0.14                | 0.42       |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD23 | 6                   | 0.37     | 0.14                | 0.42       |
| (1,2710) | 1:213:A:ASP:HB2  | 1:214:A:GLU:H    | 6                   | 0.36     | 0.08                | 0.38       |
| (1,2710) | 1:213:A:ASP:HB3  | 1:214:A:GLU:H    | 6                   | 0.36     | 0.08                | 0.38       |
| (1,2019) | 2:682:B:ILE:HG12 | 2:682:B:ILE:H    | 6                   | 0.35     | 0.03                | 0.36       |
| (1,2019) | 2:682:B:ILE:HD11 | 2:682:B:ILE:H    | 6                   | 0.35     | 0.03                | 0.36       |
| (1,2019) | 2:682:B:ILE:HD12 | 2:682:B:ILE:H    | 6                   | 0.35     | 0.03                | 0.36       |
| (1,2019) | 2:682:B:ILE:HD13 | 2:682:B:ILE:H    | 6                   | 0.35     | 0.03                | 0.36       |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD11 | 6                   | 0.32     | 0.15                | 0.28       |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD12 | 6                   | 0.32     | 0.15                | 0.28       |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD13 | 6                   | 0.32     | 0.15                | 0.28       |
| (1,174)  | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD11 | 6                   | 0.32     | 0.15                | 0.28       |
| (1,174)  | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD12 | 6                   | 0.32     | 0.15                | 0.28       |
| (1,174)  | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD13 | 6                   | 0.32     | 0.15                | 0.28       |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD21 | 6                   | 0.3      | 0.1                 | 0.32       |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD22 | 6                   | 0.3      | 0.1                 | 0.32       |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD23 | 6                   | 0.3      | 0.1                 | 0.32       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,371)  | 2:668:B:LYS:HB3  | 2:668:B:LYS:HA   | 6                   | 0.28     | 0.06                | 0.31       |
| (1,371)  | 2:647:B:GLU:HB2  | 2:647:B:GLU:HA   | 6                   | 0.28     | 0.06                | 0.31       |
| (1,371)  | 2:635:B:GLU:HB2  | 2:632:B:ARG:HA   | 6                   | 0.28     | 0.06                | 0.31       |
| (1,1559) | 2:716:B:LYS:HG2  | 2:716:B:LYS:HA   | 6                   | 0.25     | 0.18                | 0.2        |
| (1,521)  | 2:677:B:LYS:HG3  | 2:677:B:LYS:H    | 6                   | 0.23     | 0.11                | 0.2        |
| (1,521)  | 2:675:B:ALA:HB1  | 2:677:B:LYS:H    | 6                   | 0.23     | 0.11                | 0.2        |
| (1,521)  | 2:675:B:ALA:HB2  | 2:677:B:LYS:H    | 6                   | 0.23     | 0.11                | 0.2        |
| (1,521)  | 2:675:B:ALA:HB3  | 2:677:B:LYS:H    | 6                   | 0.23     | 0.11                | 0.2        |
| (1,521)  | 2:677:B:LYS:HD3  | 2:677:B:LYS:H    | 6                   | 0.23     | 0.11                | 0.2        |
| (1,416)  | 1:219:A:ASP:HA   | 2:695:B:ILE:HD11 | 6                   | 0.22     | 0.08                | 0.19       |
| (1,416)  | 1:219:A:ASP:HA   | 2:695:B:ILE:HD12 | 6                   | 0.22     | 0.08                | 0.19       |
| (1,416)  | 1:219:A:ASP:HA   | 2:695:B:ILE:HD13 | 6                   | 0.22     | 0.08                | 0.19       |
| (1,416)  | 1:222:A:THR:HA   | 2:695:B:ILE:HD11 | 6                   | 0.22     | 0.08                | 0.19       |
| (1,416)  | 1:222:A:THR:HA   | 2:695:B:ILE:HD12 | 6                   | 0.22     | 0.08                | 0.19       |
| (1,416)  | 1:222:A:THR:HA   | 2:695:B:ILE:HD13 | 6                   | 0.22     | 0.08                | 0.19       |
| (1,1520) | 2:612:B:ARG:HG3  | 2:612:B:ARG:HA   | 6                   | 0.2      | 0.06                | 0.22       |
| (1,1520) | 2:612:B:ARG:HG2  | 2:612:B:ARG:HA   | 6                   | 0.2      | 0.06                | 0.22       |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD21 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD22 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD23 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD21 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD22 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD23 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD21 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD22 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD23 | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD11 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD12 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD13 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD11 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD12 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD13 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD11 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD12 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD13 | 6                   | 0.14     | 0.01                | 0.15       |
| (1,1312) | 2:698:B:LYS:HB2  | 2:698:B:LYS:HD3  | 6                   | 0.14     | 0.03                | 0.14       |
| (1,1312) | 2:698:B:LYS:HB3  | 2:698:B:LYS:HD3  | 6                   | 0.14     | 0.03                | 0.14       |
| (1,1312) | 2:698:B:LYS:HB3  | 2:698:B:LYS:HD2  | 6                   | 0.14     | 0.03                | 0.14       |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB1  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB2  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB3  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB1  | 6                   | 0.13     | 0.02                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB2  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB3  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB1  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB2  | 6                   | 0.13     | 0.02                | 0.12       |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB3  | 6                   | 0.13     | 0.02                | 0.12       |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD11 | 5                   | 1.01     | 0.65                | 1.34       |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD12 | 5                   | 1.01     | 0.65                | 1.34       |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD13 | 5                   | 1.01     | 0.65                | 1.34       |
| (1,711)  | 1:211:A:LEU:HD11 | 2:675:B:ALA:H    | 5                   | 0.91     | 0.21                | 0.9        |
| (1,711)  | 1:211:A:LEU:HD12 | 2:675:B:ALA:H    | 5                   | 0.91     | 0.21                | 0.9        |
| (1,711)  | 1:211:A:LEU:HD13 | 2:675:B:ALA:H    | 5                   | 0.91     | 0.21                | 0.9        |
| (1,711)  | 2:670:B:LEU:HD21 | 2:675:B:ALA:H    | 5                   | 0.91     | 0.21                | 0.9        |
| (1,711)  | 2:670:B:LEU:HD22 | 2:675:B:ALA:H    | 5                   | 0.91     | 0.21                | 0.9        |
| (1,711)  | 2:670:B:LEU:HD23 | 2:675:B:ALA:H    | 5                   | 0.91     | 0.21                | 0.9        |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD21 | 5                   | 0.81     | 0.59                | 0.87       |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD22 | 5                   | 0.81     | 0.59                | 0.87       |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD23 | 5                   | 0.81     | 0.59                | 0.87       |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD21 | 5                   | 0.77     | 0.46                | 0.55       |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD22 | 5                   | 0.77     | 0.46                | 0.55       |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD23 | 5                   | 0.77     | 0.46                | 0.55       |
| (1,765)  | 1:208:A:ASN:HB3  | 1:210:A:LEU:HD21 | 5                   | 0.77     | 0.46                | 0.55       |
| (1,765)  | 1:208:A:ASN:HB3  | 1:210:A:LEU:HD22 | 5                   | 0.77     | 0.46                | 0.55       |
| (1,765)  | 1:208:A:ASN:HB3  | 1:210:A:LEU:HD23 | 5                   | 0.77     | 0.46                | 0.55       |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD21 | 5                   | 0.75     | 0.19                | 0.8        |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD22 | 5                   | 0.75     | 0.19                | 0.8        |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD23 | 5                   | 0.75     | 0.19                | 0.8        |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD11 | 5                   | 0.72     | 0.02                | 0.72       |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD12 | 5                   | 0.72     | 0.02                | 0.72       |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD13 | 5                   | 0.72     | 0.02                | 0.72       |
| (1,238)  | 2:646:B:ALA:HB1  | 2:647:B:GLU:HG2  | 5                   | 0.7      | 0.22                | 0.8        |
| (1,238)  | 2:646:B:ALA:HB2  | 2:647:B:GLU:HG2  | 5                   | 0.7      | 0.22                | 0.8        |
| (1,238)  | 2:646:B:ALA:HB3  | 2:647:B:GLU:HG2  | 5                   | 0.7      | 0.22                | 0.8        |
| (1,238)  | 2:716:B:LYS:HG3  | 2:720:B:GLU:HG3  | 5                   | 0.7      | 0.22                | 0.8        |
| (1,238)  | 2:646:B:ALA:HB1  | 2:647:B:GLU:HG3  | 5                   | 0.7      | 0.22                | 0.8        |
| (1,238)  | 2:646:B:ALA:HB2  | 2:647:B:GLU:HG3  | 5                   | 0.7      | 0.22                | 0.8        |
| (1,238)  | 2:646:B:ALA:HB3  | 2:647:B:GLU:HG3  | 5                   | 0.7      | 0.22                | 0.8        |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG11 | 5                   | 0.69     | 0.29                | 0.62       |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG12 | 5                   | 0.69     | 0.29                | 0.62       |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG13 | 5                   | 0.69     | 0.29                | 0.62       |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD21 | 5                   | 0.63     | 0.32                | 0.66       |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD22 | 5                   | 0.63     | 0.32                | 0.66       |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD23 | 5                   | 0.63     | 0.32                | 0.66       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD21 | 5                   | 0.63     | 0.32                | 0.66       |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD22 | 5                   | 0.63     | 0.32                | 0.66       |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD23 | 5                   | 0.63     | 0.32                | 0.66       |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD21 | 5                   | 0.55     | 0.33                | 0.41       |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD22 | 5                   | 0.55     | 0.33                | 0.41       |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD23 | 5                   | 0.55     | 0.33                | 0.41       |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD21 | 5                   | 0.55     | 0.33                | 0.41       |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD22 | 5                   | 0.55     | 0.33                | 0.41       |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD23 | 5                   | 0.55     | 0.33                | 0.41       |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD11 | 5                   | 0.53     | 0.0                 | 0.53       |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD12 | 5                   | 0.53     | 0.0                 | 0.53       |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD13 | 5                   | 0.53     | 0.0                 | 0.53       |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE1  | 5                   | 0.51     | 0.11                | 0.46       |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE2  | 5                   | 0.51     | 0.11                | 0.46       |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE3  | 5                   | 0.51     | 0.11                | 0.46       |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB1  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB2  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB3  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB1  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB2  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB3  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB1  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB2  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB3  | 5                   | 0.51     | 0.19                | 0.58       |
| (1,756)  | 2:620:B:LEU:HD21 | 2:707:B:TRP:HE1  | 5                   | 0.48     | 0.32                | 0.37       |
| (1,756)  | 2:620:B:LEU:HD22 | 2:707:B:TRP:HE1  | 5                   | 0.48     | 0.32                | 0.37       |
| (1,756)  | 2:620:B:LEU:HD23 | 2:707:B:TRP:HE1  | 5                   | 0.48     | 0.32                | 0.37       |
| (1,175)  | 2:640:B:LYS:HD3  | 2:637:B:ILE:HD11 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:640:B:LYS:HD3  | 2:637:B:ILE:HD12 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:640:B:LYS:HD3  | 2:637:B:ILE:HD13 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:640:B:LYS:HD2  | 2:637:B:ILE:HD11 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:640:B:LYS:HD2  | 2:637:B:ILE:HD12 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:640:B:LYS:HD2  | 2:637:B:ILE:HD13 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD11 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD12 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD13 | 5                   | 0.48     | 0.34                | 0.35       |
| (1,536)  | 2:614:B:GLU:HB2  | 2:615:B:ASP:H    | 5                   | 0.45     | 0.23                | 0.34       |
| (1,536)  | 2:634:B:LEU:HG   | 2:634:B:LEU:H    | 5                   | 0.45     | 0.23                | 0.34       |
| (1,1423) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HG3  | 5                   | 0.43     | 0.12                | 0.39       |
| (1,1423) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HG3  | 5                   | 0.43     | 0.12                | 0.39       |
| (1,1423) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HG3  | 5                   | 0.43     | 0.12                | 0.39       |
| (1,316)  | 2:629:B:ALA:HA   | 2:632:B:ARG:HD2  | 5                   | 0.41     | 0.19                | 0.32       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,316) | 2:716:B:LYS:HA   | 2:719:B:ARG:HD2  | 5                   | 0.41     | 0.19                | 0.32       |
| (1,316) | 2:716:B:LYS:HA   | 2:719:B:ARG:HD3  | 5                   | 0.41     | 0.19                | 0.32       |
| (2,13)  | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD21 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD22 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD23 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD21 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD22 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD23 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD21 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD22 | 5                   | 0.41     | 0.13                | 0.4        |
| (2,13)  | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD23 | 5                   | 0.41     | 0.13                | 0.4        |
| (1,282) | 2:610:B:ILE:HD11 | 2:608:B:GLU:HG3  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 2:610:B:ILE:HD12 | 2:608:B:GLU:HG3  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 2:610:B:ILE:HD13 | 2:608:B:GLU:HG3  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 1:207:A:LEU:HD11 | 2:616:B:GLU:HG3  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 1:207:A:LEU:HD12 | 2:616:B:GLU:HG3  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 1:207:A:LEU:HD13 | 2:616:B:GLU:HG3  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 2:610:B:ILE:HD11 | 2:608:B:GLU:HG2  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 2:610:B:ILE:HD12 | 2:608:B:GLU:HG2  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,282) | 2:610:B:ILE:HD13 | 2:608:B:GLU:HG2  | 5                   | 0.4      | 0.21                | 0.46       |
| (1,169) | 2:634:B:LEU:HB2  | 2:700:B:LEU:HD21 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:634:B:LEU:HB2  | 2:700:B:LEU:HD22 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:634:B:LEU:HB2  | 2:700:B:LEU:HD23 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD21 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD22 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD23 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:670:B:LEU:HB2  | 2:700:B:LEU:HD21 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:670:B:LEU:HB2  | 2:700:B:LEU:HD22 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,169) | 2:670:B:LEU:HB2  | 2:700:B:LEU:HD23 | 5                   | 0.37     | 0.23                | 0.3        |
| (1,667) | 1:220:A:LEU:HD21 | 2:677:B:LYS:H    | 5                   | 0.37     | 0.05                | 0.37       |
| (1,667) | 1:220:A:LEU:HD22 | 2:677:B:LYS:H    | 5                   | 0.37     | 0.05                | 0.37       |
| (1,667) | 1:220:A:LEU:HD23 | 2:677:B:LYS:H    | 5                   | 0.37     | 0.05                | 0.37       |
| (1,667) | 1:210:A:LEU:HD21 | 2:677:B:LYS:H    | 5                   | 0.37     | 0.05                | 0.37       |
| (1,667) | 1:210:A:LEU:HD22 | 2:677:B:LYS:H    | 5                   | 0.37     | 0.05                | 0.37       |
| (1,667) | 1:210:A:LEU:HD23 | 2:677:B:LYS:H    | 5                   | 0.37     | 0.05                | 0.37       |
| (1,151) | 2:641:B:LEU:HG   | 2:654:B:LEU:HD11 | 5                   | 0.36     | 0.18                | 0.42       |
| (1,151) | 2:641:B:LEU:HG   | 2:654:B:LEU:HD12 | 5                   | 0.36     | 0.18                | 0.42       |
| (1,151) | 2:641:B:LEU:HG   | 2:654:B:LEU:HD13 | 5                   | 0.36     | 0.18                | 0.42       |
| (1,151) | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD11 | 5                   | 0.36     | 0.18                | 0.42       |
| (1,151) | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD12 | 5                   | 0.36     | 0.18                | 0.42       |
| (1,151) | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD13 | 5                   | 0.36     | 0.18                | 0.42       |
| (1,61)  | 2:632:B:ARG:HA   | 2:632:B:ARG:HG3  | 5                   | 0.36     | 0.07                | 0.4        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,61)   | 2:629:B:ALA:HA   | 2:632:B:ARG:HG3  | 5                   | 0.36     | 0.07                | 0.4        |
| (1,444)  | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD21 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD22 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD23 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:670:B:LEU:HG   | 2:658:B:LEU:HD21 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:670:B:LEU:HG   | 2:658:B:LEU:HD22 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:670:B:LEU:HG   | 2:658:B:LEU:HD23 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:633:B:VAL:HB   | 2:658:B:LEU:HD21 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:633:B:VAL:HB   | 2:658:B:LEU:HD22 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,444)  | 2:633:B:VAL:HB   | 2:658:B:LEU:HD23 | 5                   | 0.35     | 0.16                | 0.34       |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD21 | 5                   | 0.34     | 0.14                | 0.41       |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD22 | 5                   | 0.34     | 0.14                | 0.41       |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD23 | 5                   | 0.34     | 0.14                | 0.41       |
| (1,1873) | 2:608:B:GLU:HB2  | 2:608:B:GLU:H    | 5                   | 0.3      | 0.1                 | 0.32       |
| (1,242)  | 2:692:B:ALA:HB1  | 2:688:B:ASN:HB2  | 5                   | 0.29     | 0.07                | 0.28       |
| (1,242)  | 2:692:B:ALA:HB2  | 2:688:B:ASN:HB2  | 5                   | 0.29     | 0.07                | 0.28       |
| (1,242)  | 2:692:B:ALA:HB3  | 2:688:B:ASN:HB2  | 5                   | 0.29     | 0.07                | 0.28       |
| (1,242)  | 2:673:B:ILE:HG21 | 2:674:B:TYR:HB2  | 5                   | 0.29     | 0.07                | 0.28       |
| (1,242)  | 2:673:B:ILE:HG22 | 2:674:B:TYR:HB2  | 5                   | 0.29     | 0.07                | 0.28       |
| (1,242)  | 2:673:B:ILE:HG23 | 2:674:B:TYR:HB2  | 5                   | 0.29     | 0.07                | 0.28       |
| (1,2112) | 2:644:B:LEU:HD21 | 2:652:B:PHE:H    | 5                   | 0.29     | 0.1                 | 0.35       |
| (1,2112) | 2:644:B:LEU:HD22 | 2:652:B:PHE:H    | 5                   | 0.29     | 0.1                 | 0.35       |
| (1,2112) | 2:644:B:LEU:HD23 | 2:652:B:PHE:H    | 5                   | 0.29     | 0.1                 | 0.35       |
| (1,2749) | 1:221:A:ARG:HG3  | 1:221:A:ARG:H    | 5                   | 0.27     | 0.15                | 0.31       |
| (1,1783) | 2:727:B:LEU:HB2  | 2:727:B:LEU:H    | 5                   | 0.27     | 0.02                | 0.27       |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE1  | 5                   | 0.23     | 0.1                 | 0.25       |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE2  | 5                   | 0.23     | 0.1                 | 0.25       |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE3  | 5                   | 0.23     | 0.1                 | 0.25       |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE1  | 5                   | 0.23     | 0.1                 | 0.25       |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE2  | 5                   | 0.23     | 0.1                 | 0.25       |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE3  | 5                   | 0.23     | 0.1                 | 0.25       |
| (1,1838) | 2:615:B:ASP:HB2  | 2:616:B:GLU:H    | 5                   | 0.2      | 0.07                | 0.21       |
| (1,1672) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HE3  | 5                   | 0.19     | 0.06                | 0.16       |
| (1,1672) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HE3  | 5                   | 0.19     | 0.06                | 0.16       |
| (1,1672) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HE3  | 5                   | 0.19     | 0.06                | 0.16       |
| (1,1672) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HE2  | 5                   | 0.19     | 0.06                | 0.16       |
| (1,1672) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HE2  | 5                   | 0.19     | 0.06                | 0.16       |
| (1,1672) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HE2  | 5                   | 0.19     | 0.06                | 0.16       |
| (1,1891) | 2:612:B:ARG:HB2  | 2:612:B:ARG:H    | 5                   | 0.18     | 0.05                | 0.2        |
| (1,2694) | 1:210:A:LEU:HB3  | 1:210:A:LEU:H    | 5                   | 0.16     | 0.04                | 0.16       |
| (1,1561) | 2:716:B:LYS:HD2  | 2:716:B:LYS:HA   | 5                   | 0.16     | 0.07                | 0.13       |
| (1,1561) | 2:716:B:LYS:HD3  | 2:716:B:LYS:HA   | 5                   | 0.16     | 0.07                | 0.13       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,624)  | 2:647:B:GLU:HB2  | 2:648:B:GLU:H    | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD21 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD22 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD23 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,218)  | 2:698:B:LYS:HE2  | 2:698:B:LYS:HD3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,218)  | 2:716:B:LYS:HE2  | 2:716:B:LYS:HD3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,218)  | 2:728:B:LYS:HE2  | 2:728:B:LYS:HD3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,218)  | 2:728:B:LYS:HE3  | 2:728:B:LYS:HD3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,218)  | 2:728:B:LYS:HE3  | 2:728:B:LYS:HD2  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD21 | 4                   | 1.68     | 0.96                | 1.58       |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD22 | 4                   | 1.68     | 0.96                | 1.58       |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD23 | 4                   | 1.68     | 0.96                | 1.58       |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD11 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD12 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD13 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD11 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD12 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD13 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD11 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD12 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD13 | 4                   | 1.01     | 0.4                 | 0.98       |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD11 | 4                   | 0.73     | 0.36                | 0.66       |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD12 | 4                   | 0.73     | 0.36                | 0.66       |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD13 | 4                   | 0.73     | 0.36                | 0.66       |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD11 | 4                   | 0.73     | 0.36                | 0.66       |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD12 | 4                   | 0.73     | 0.36                | 0.66       |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD13 | 4                   | 0.73     | 0.36                | 0.66       |
| (1,237)  | 2:613:B:CYS:HB2  | 2:616:B:GLU:HG3  | 4                   | 0.71     | 0.46                | 0.68       |
| (1,237)  | 2:613:B:CYS:HB3  | 2:614:B:GLU:HG3  | 4                   | 0.71     | 0.46                | 0.68       |
| (1,237)  | 2:613:B:CYS:HB3  | 2:614:B:GLU:HG2  | 4                   | 0.71     | 0.46                | 0.68       |
| (1,659)  | 2:670:B:LEU:HD21 | 2:674:B:TYR:H    | 4                   | 0.63     | 0.39                | 0.58       |
| (1,659)  | 2:670:B:LEU:HD22 | 2:674:B:TYR:H    | 4                   | 0.63     | 0.39                | 0.58       |
| (1,659)  | 2:670:B:LEU:HD23 | 2:674:B:TYR:H    | 4                   | 0.63     | 0.39                | 0.58       |
| (1,659)  | 1:211:A:LEU:HD11 | 2:674:B:TYR:H    | 4                   | 0.63     | 0.39                | 0.58       |
| (1,659)  | 1:211:A:LEU:HD12 | 2:674:B:TYR:H    | 4                   | 0.63     | 0.39                | 0.58       |
| (1,659)  | 1:211:A:LEU:HD13 | 2:674:B:TYR:H    | 4                   | 0.63     | 0.39                | 0.58       |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE1  | 4                   | 0.6      | 0.3                 | 0.64       |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE2  | 4                   | 0.6      | 0.3                 | 0.64       |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE3  | 4                   | 0.6      | 0.3                 | 0.64       |
| (1,2058) | 2:645:B:SER:HB2  | 2:645:B:SER:H    | 4                   | 0.51     | 0.01                | 0.5        |
| (1,155)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD11 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,155)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD12 | 4                   | 0.48     | 0.19                | 0.45       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,155)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD13 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,155)  | 2:638:B:GLN:HB3  | 2:641:B:LEU:HD11 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,155)  | 2:638:B:GLN:HB3  | 2:641:B:LEU:HD12 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,155)  | 2:638:B:GLN:HB3  | 2:641:B:LEU:HD13 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,155)  | 2:638:B:GLN:HG3  | 2:641:B:LEU:HD11 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,155)  | 2:638:B:GLN:HG3  | 2:641:B:LEU:HD12 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,155)  | 2:638:B:GLN:HG3  | 2:641:B:LEU:HD13 | 4                   | 0.48     | 0.19                | 0.45       |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD21 | 4                   | 0.46     | 0.12                | 0.42       |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD22 | 4                   | 0.46     | 0.12                | 0.42       |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD23 | 4                   | 0.46     | 0.12                | 0.42       |
| (1,466)  | 2:654:B:LEU:HA   | 2:659:B:GLY:H    | 4                   | 0.4      | 0.17                | 0.47       |
| (1,466)  | 2:726:B:TYR:HA   | 2:728:B:LYS:H    | 4                   | 0.4      | 0.17                | 0.47       |
| (1,466)  | 2:655:B:ASP:HA   | 2:659:B:GLY:H    | 4                   | 0.4      | 0.17                | 0.47       |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD21 | 4                   | 0.4      | 0.19                | 0.34       |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD22 | 4                   | 0.4      | 0.19                | 0.34       |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD23 | 4                   | 0.4      | 0.19                | 0.34       |
| (1,464)  | 2:647:B:GLU:HA   | 2:649:B:GLN:HE21 | 4                   | 0.39     | 0.07                | 0.41       |
| (1,464)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE21 | 4                   | 0.39     | 0.07                | 0.41       |
| (1,88)   | 2:647:B:GLU:HA   | 2:647:B:GLU:HG2  | 4                   | 0.39     | 0.02                | 0.4        |
| (1,88)   | 2:647:B:GLU:HA   | 2:647:B:GLU:HG3  | 4                   | 0.39     | 0.02                | 0.4        |
| (1,1570) | 2:647:B:GLU:HG2  | 2:647:B:GLU:HA   | 4                   | 0.39     | 0.02                | 0.4        |
| (1,1570) | 2:647:B:GLU:HG3  | 2:647:B:GLU:HA   | 4                   | 0.39     | 0.02                | 0.4        |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD21 | 4                   | 0.39     | 0.28                | 0.34       |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD22 | 4                   | 0.39     | 0.28                | 0.34       |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD23 | 4                   | 0.39     | 0.28                | 0.34       |
| (1,170)  | 2:634:B:LEU:HG   | 2:700:B:LEU:HD21 | 4                   | 0.39     | 0.28                | 0.34       |
| (1,170)  | 2:634:B:LEU:HG   | 2:700:B:LEU:HD22 | 4                   | 0.39     | 0.28                | 0.34       |
| (1,170)  | 2:634:B:LEU:HG   | 2:700:B:LEU:HD23 | 4                   | 0.39     | 0.28                | 0.34       |
| (1,420)  | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD11 | 4                   | 0.39     | 0.16                | 0.46       |
| (1,420)  | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD12 | 4                   | 0.39     | 0.16                | 0.46       |
| (1,420)  | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD13 | 4                   | 0.39     | 0.16                | 0.46       |
| (1,420)  | 2:682:B:ILE:HG13 | 2:681:B:ILE:HD11 | 4                   | 0.39     | 0.16                | 0.46       |
| (1,420)  | 2:682:B:ILE:HG13 | 2:681:B:ILE:HD12 | 4                   | 0.39     | 0.16                | 0.46       |
| (1,420)  | 2:682:B:ILE:HG13 | 2:681:B:ILE:HD13 | 4                   | 0.39     | 0.16                | 0.46       |
| (1,2125) | 2:613:B:CYS:HB3  | 2:615:B:ASP:H    | 4                   | 0.36     | 0.12                | 0.3        |
| (1,2125) | 2:613:B:CYS:HB2  | 2:615:B:ASP:H    | 4                   | 0.36     | 0.12                | 0.3        |
| (1,2463) | 2:621:B:ASP:HA   | 2:711:B:GLN:HE22 | 4                   | 0.31     | 0.11                | 0.3        |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB1  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB2  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB3  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB1  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB2  | 4                   | 0.31     | 0.14                | 0.28       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB3  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB1  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB2  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB3  | 4                   | 0.31     | 0.14                | 0.28       |
| (1,697)  | 2:687:B:LYS:HD2  | 2:688:B:ASN:H    | 4                   | 0.3      | 0.11                | 0.27       |
| (1,697)  | 2:687:B:LYS:HD3  | 2:688:B:ASN:H    | 4                   | 0.3      | 0.11                | 0.27       |
| (1,998)  | 2:695:B:ILE:HA   | 2:698:B:LYS:HD3  | 4                   | 0.29     | 0.12                | 0.24       |
| (1,998)  | 2:695:B:ILE:HA   | 2:698:B:LYS:HD2  | 4                   | 0.29     | 0.12                | 0.24       |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD11 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD12 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD13 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD11 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD12 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD13 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD11 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD12 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD13 | 4                   | 0.27     | 0.11                | 0.26       |
| (1,295)  | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB1  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB2  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB3  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB1  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB2  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB3  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB1  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB2  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB3  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB1  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB2  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB3  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB1  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB2  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB3  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB1  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB2  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,295)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB3  | 4                   | 0.26     | 0.14                | 0.22       |
| (1,609)  | 2:700:B:LEU:HB3  | 2:701:B:LYS:H    | 4                   | 0.24     | 0.03                | 0.24       |
| (1,609)  | 2:641:B:LEU:HB3  | 2:641:B:LEU:H    | 4                   | 0.24     | 0.03                | 0.24       |
| (1,920)  | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD21 | 4                   | 0.24     | 0.07                | 0.23       |
| (1,920)  | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD22 | 4                   | 0.24     | 0.07                | 0.23       |
| (1,920)  | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD23 | 4                   | 0.24     | 0.07                | 0.23       |
| (1,1289) | 2:689:B:PRO:HB3  | 2:653:B:ARG:HG3  | 4                   | 0.23     | 0.07                | 0.19       |
| (1,637)  | 2:633:B:VAL:HG21 | 2:658:B:LEU:H    | 4                   | 0.22     | 0.06                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,637)  | 2:633:B:VAL:HG22 | 2:658:B:LEU:H    | 4                   | 0.22     | 0.06                | 0.2        |
| (1,637)  | 2:633:B:VAL:HG23 | 2:658:B:LEU:H    | 4                   | 0.22     | 0.06                | 0.2        |
| (1,637)  | 2:654:B:LEU:HD21 | 2:658:B:LEU:H    | 4                   | 0.22     | 0.06                | 0.2        |
| (1,637)  | 2:654:B:LEU:HD22 | 2:658:B:LEU:H    | 4                   | 0.22     | 0.06                | 0.2        |
| (1,637)  | 2:654:B:LEU:HD23 | 2:658:B:LEU:H    | 4                   | 0.22     | 0.06                | 0.2        |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD11 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD12 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD13 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,921)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD11 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,921)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD12 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,921)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD13 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,1911) | 2:724:B:LYS:HB3  | 2:724:B:LYS:H    | 4                   | 0.22     | 0.05                | 0.23       |
| (1,1911) | 2:724:B:LYS:HB2  | 2:724:B:LYS:H    | 4                   | 0.22     | 0.05                | 0.23       |
| (1,388)  | 2:694:B:PRO:HB3  | 2:698:B:LYS:HE3  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,388)  | 2:648:B:GLU:HB3  | 2:651:B:LYS:HE2  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,2046) | 2:643:B:ARG:HG2  | 2:643:B:ARG:H    | 4                   | 0.2      | 0.1                 | 0.18       |
| (1,467)  | 2:725:B:TYR:HB3  | 2:726:B:TYR:H    | 4                   | 0.2      | 0.03                | 0.18       |
| (1,467)  | 2:726:B:TYR:HB3  | 2:726:B:TYR:H    | 4                   | 0.2      | 0.03                | 0.18       |
| (1,122)  | 2:672:B:ARG:HG2  | 2:623:B:VAL:HG21 | 4                   | 0.17     | 0.05                | 0.18       |
| (1,122)  | 2:672:B:ARG:HG2  | 2:623:B:VAL:HG22 | 4                   | 0.17     | 0.05                | 0.18       |
| (1,122)  | 2:672:B:ARG:HG2  | 2:623:B:VAL:HG23 | 4                   | 0.17     | 0.05                | 0.18       |
| (1,122)  | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG21 | 4                   | 0.17     | 0.05                | 0.18       |
| (1,122)  | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG22 | 4                   | 0.17     | 0.05                | 0.18       |
| (1,122)  | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG23 | 4                   | 0.17     | 0.05                | 0.18       |
| (1,2779) | 1:226:A:LEU:HB2  | 1:226:A:LEU:H    | 4                   | 0.17     | 0.04                | 0.16       |
| (1,1353) | 2:647:B:GLU:HB2  | 2:647:B:GLU:HG2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,1353) | 2:647:B:GLU:HB2  | 2:647:B:GLU:HG3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2478) | 1:207:A:LEU:HD21 | 1:207:A:LEU:HA   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,2478) | 1:207:A:LEU:HD22 | 1:207:A:LEU:HA   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,2478) | 1:207:A:LEU:HD23 | 1:207:A:LEU:HA   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,2478) | 1:207:A:LEU:HD11 | 1:207:A:LEU:HA   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,2478) | 1:207:A:LEU:HD12 | 1:207:A:LEU:HA   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,2478) | 1:207:A:LEU:HD13 | 1:207:A:LEU:HA   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,422)  | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD11 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD12 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD13 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD11 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD12 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD13 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD11 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD12 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,422)  | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD13 | 4                   | 0.14     | 0.04                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG21 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG22 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG23 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG21 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG22 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG23 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG21 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG22 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG23 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,2278) | 2:689:B:PRO:HG2  | 2:688:B:ASN:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD11 | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD12 | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD13 | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD21 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD22 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD23 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,658)  | 2:670:B:LEU:HD11 | 2:674:B:TYR:H    | 3                   | 1.16     | 0.05                | 1.16       |
| (1,658)  | 2:670:B:LEU:HD12 | 2:674:B:TYR:H    | 3                   | 1.16     | 0.05                | 1.16       |
| (1,658)  | 2:670:B:LEU:HD13 | 2:674:B:TYR:H    | 3                   | 1.16     | 0.05                | 1.16       |
| (1,855)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD3  | 3                   | 1.15     | 0.1                 | 1.21       |
| (1,855)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD3  | 3                   | 1.15     | 0.1                 | 1.21       |
| (1,855)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD3  | 3                   | 1.15     | 0.1                 | 1.21       |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD21 | 3                   | 1.08     | 0.64                | 0.92       |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD22 | 3                   | 1.08     | 0.64                | 0.92       |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD23 | 3                   | 1.08     | 0.64                | 0.92       |
| (1,656)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:H    | 3                   | 1.06     | 0.34                | 1.28       |
| (1,656)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:H    | 3                   | 1.06     | 0.34                | 1.28       |
| (1,656)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:H    | 3                   | 1.06     | 0.34                | 1.28       |
| (1,656)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:H    | 3                   | 1.06     | 0.34                | 1.28       |
| (1,656)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:H    | 3                   | 1.06     | 0.34                | 1.28       |
| (1,656)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:H    | 3                   | 1.06     | 0.34                | 1.28       |
| (1,178)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:HD11 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:HD12 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:HD13 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:HD11 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:HD12 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:HD13 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:HD11 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:HD12 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:HD13 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD11 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD12 | 3                   | 0.94     | 0.36                | 1.02       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,178)  | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD13 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD11 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD12 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD13 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD11 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD12 | 3                   | 0.94     | 0.36                | 1.02       |
| (1,178)  | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD13 | 3                   | 0.94     | 0.36                | 1.02       |
| (2,14)   | 1:220:A:LEU:HD21 | 1:217:A:MET:HG2  | 3                   | 0.77     | 0.39                | 0.52       |
| (2,14)   | 1:220:A:LEU:HD22 | 1:217:A:MET:HG2  | 3                   | 0.77     | 0.39                | 0.52       |
| (2,14)   | 1:220:A:LEU:HD23 | 1:217:A:MET:HG2  | 3                   | 0.77     | 0.39                | 0.52       |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD11 | 3                   | 0.76     | 0.12                | 0.8        |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD12 | 3                   | 0.76     | 0.12                | 0.8        |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD13 | 3                   | 0.76     | 0.12                | 0.8        |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD11 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD12 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD13 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD11 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD12 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD13 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD11 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD12 | 3                   | 0.74     | 0.31                | 0.92       |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD13 | 3                   | 0.74     | 0.31                | 0.92       |
| (2,18)   | 1:220:A:LEU:HD21 | 1:221:A:ARG:HG2  | 3                   | 0.72     | 0.32                | 0.91       |
| (2,18)   | 1:220:A:LEU:HD22 | 1:221:A:ARG:HG2  | 3                   | 0.72     | 0.32                | 0.91       |
| (2,18)   | 1:220:A:LEU:HD23 | 1:221:A:ARG:HG2  | 3                   | 0.72     | 0.32                | 0.91       |
| (1,187)  | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG11 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG12 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG13 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG11 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG12 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG13 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG11 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG12 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG13 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HG11 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HG12 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HG13 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HG11 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HG12 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HG13 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HG11 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,187)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HG12 | 3                   | 0.66     | 0.3                 | 0.63       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,187)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HG13 | 3                   | 0.66     | 0.3                 | 0.63       |
| (1,317)  | 2:712:B:ARG:HA   | 2:712:B:ARG:HD2  | 3                   | 0.64     | 0.17                | 0.74       |
| (1,2590) | 2:677:B:LYS:HB2  | 1:220:A:LEU:HD11 | 3                   | 0.64     | 0.6                 | 0.33       |
| (1,2590) | 2:677:B:LYS:HB2  | 1:220:A:LEU:HD12 | 3                   | 0.64     | 0.6                 | 0.33       |
| (1,2590) | 2:677:B:LYS:HB2  | 1:220:A:LEU:HD13 | 3                   | 0.64     | 0.6                 | 0.33       |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD11 | 3                   | 0.64     | 0.6                 | 0.33       |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD12 | 3                   | 0.64     | 0.6                 | 0.33       |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD13 | 3                   | 0.64     | 0.6                 | 0.33       |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD21 | 3                   | 0.6      | 0.3                 | 0.4        |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD22 | 3                   | 0.6      | 0.3                 | 0.4        |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD23 | 3                   | 0.6      | 0.3                 | 0.4        |
| (1,1740) | 2:691:B:ILE:HG12 | 2:688:B:ASN:HD22 | 3                   | 0.57     | 0.37                | 0.55       |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG21 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG22 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG23 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG21 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG22 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG23 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG21 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG22 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG23 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD11 | 2:673:B:ILE:HG21 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD11 | 2:673:B:ILE:HG22 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD11 | 2:673:B:ILE:HG23 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD12 | 2:673:B:ILE:HG21 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD12 | 2:673:B:ILE:HG22 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD12 | 2:673:B:ILE:HG23 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD13 | 2:673:B:ILE:HG21 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD13 | 2:673:B:ILE:HG22 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,418)  | 1:210:A:LEU:HD13 | 2:673:B:ILE:HG23 | 3                   | 0.56     | 0.05                | 0.56       |
| (1,1892) | 2:612:B:ARG:HG2  | 2:612:B:ARG:H    | 3                   | 0.51     | 0.09                | 0.47       |
| (1,265)  | 2:697:B:LEU:HD21 | 2:638:B:GLN:HB2  | 3                   | 0.46     | 0.19                | 0.43       |
| (1,265)  | 2:697:B:LEU:HD22 | 2:638:B:GLN:HB2  | 3                   | 0.46     | 0.19                | 0.43       |
| (1,265)  | 2:697:B:LEU:HD23 | 2:638:B:GLN:HB2  | 3                   | 0.46     | 0.19                | 0.43       |
| (1,937)  | 2:669:B:ALA:HA   | 2:668:B:LYS:HG3  | 3                   | 0.46     | 0.12                | 0.54       |
| (1,1626) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HA   | 3                   | 0.43     | 0.09                | 0.38       |
| (1,1626) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HA   | 3                   | 0.43     | 0.09                | 0.38       |
| (1,1626) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HA   | 3                   | 0.43     | 0.09                | 0.38       |
| (1,1351) | 2:716:B:LYS:HE2  | 2:720:B:GLU:HG3  | 3                   | 0.41     | 0.2                 | 0.51       |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD11 | 3                   | 0.41     | 0.18                | 0.52       |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD12 | 3                   | 0.41     | 0.18                | 0.52       |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD13 | 3                   | 0.41     | 0.18                | 0.52       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD11 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD12 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD13 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD11 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD12 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD13 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD11 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD12 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD13 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG21 | 2:658:B:LEU:HD11 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG21 | 2:658:B:LEU:HD12 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG21 | 2:658:B:LEU:HD13 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG22 | 2:658:B:LEU:HD11 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG22 | 2:658:B:LEU:HD12 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG22 | 2:658:B:LEU:HD13 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG23 | 2:658:B:LEU:HD11 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG23 | 2:658:B:LEU:HD12 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,150)  | 2:657:B:THR:HG23 | 2:658:B:LEU:HD13 | 3                   | 0.39     | 0.14                | 0.37       |
| (1,1710) | 2:625:B:GLU:HA   | 2:625:B:GLU:HG3  | 3                   | 0.37     | 0.03                | 0.37       |
| (1,106)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HG21 | 3                   | 0.36     | 0.18                | 0.46       |
| (1,106)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HG22 | 3                   | 0.36     | 0.18                | 0.46       |
| (1,106)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HG23 | 3                   | 0.36     | 0.18                | 0.46       |
| (1,106)  | 2:626:B:THR:HA   | 2:665:B:ILE:HG21 | 3                   | 0.36     | 0.18                | 0.46       |
| (1,106)  | 2:626:B:THR:HA   | 2:665:B:ILE:HG22 | 3                   | 0.36     | 0.18                | 0.46       |
| (1,106)  | 2:626:B:THR:HA   | 2:665:B:ILE:HG23 | 3                   | 0.36     | 0.18                | 0.46       |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD11 | 3                   | 0.36     | 0.3                 | 0.2        |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD12 | 3                   | 0.36     | 0.3                 | 0.2        |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD13 | 3                   | 0.36     | 0.3                 | 0.2        |
| (1,939)  | 2:639:B:LYS:HA   | 2:639:B:LYS:HG3  | 3                   | 0.36     | 0.08                | 0.33       |
| (1,2557) | 1:220:A:LEU:HD21 | 1:217:A:MET:HA   | 3                   | 0.35     | 0.14                | 0.44       |
| (1,2557) | 1:220:A:LEU:HD22 | 1:217:A:MET:HA   | 3                   | 0.35     | 0.14                | 0.44       |
| (1,2557) | 1:220:A:LEU:HD23 | 1:217:A:MET:HA   | 3                   | 0.35     | 0.14                | 0.44       |
| (1,409)  | 2:620:B:LEU:HD11 | 2:711:B:GLN:HA   | 3                   | 0.33     | 0.11                | 0.35       |
| (1,409)  | 2:620:B:LEU:HD12 | 2:711:B:GLN:HA   | 3                   | 0.33     | 0.11                | 0.35       |
| (1,409)  | 2:620:B:LEU:HD13 | 2:711:B:GLN:HA   | 3                   | 0.33     | 0.11                | 0.35       |
| (1,409)  | 2:697:B:LEU:HD11 | 2:697:B:LEU:HA   | 3                   | 0.33     | 0.11                | 0.35       |
| (1,409)  | 2:697:B:LEU:HD12 | 2:697:B:LEU:HA   | 3                   | 0.33     | 0.11                | 0.35       |
| (1,409)  | 2:697:B:LEU:HD13 | 2:697:B:LEU:HA   | 3                   | 0.33     | 0.11                | 0.35       |
| (1,1004) | 2:712:B:ARG:HD2  | 2:712:B:ARG:HB2  | 3                   | 0.32     | 0.17                | 0.27       |
| (1,1026) | 2:706:B:GLU:HA   | 2:709:B:GLU:HG3  | 3                   | 0.32     | 0.17                | 0.32       |
| (1,1026) | 2:706:B:GLU:HA   | 2:709:B:GLU:HG2  | 3                   | 0.32     | 0.17                | 0.32       |
| (1,2239) | 2:687:B:LYS:HE2  | 2:684:B:GLY:H    | 3                   | 0.3      | 0.18                | 0.28       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD11 | 3                   | 0.3      | 0.11                | 0.27       |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD12 | 3                   | 0.3      | 0.11                | 0.27       |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD13 | 3                   | 0.3      | 0.11                | 0.27       |
| (1,240)  | 2:716:B:LYS:HG2  | 2:720:B:GLU:HG2  | 3                   | 0.28     | 0.12                | 0.36       |
| (1,17)   | 2:624:B:LEU:HD21 | 2:708:B:ARG:HD3  | 3                   | 0.28     | 0.04                | 0.29       |
| (1,17)   | 2:624:B:LEU:HD22 | 2:708:B:ARG:HD3  | 3                   | 0.28     | 0.04                | 0.29       |
| (1,17)   | 2:624:B:LEU:HD23 | 2:708:B:ARG:HD3  | 3                   | 0.28     | 0.04                | 0.29       |
| (1,477)  | 2:712:B:ARG:HA   | 2:715:B:ASN:H    | 3                   | 0.27     | 0.12                | 0.19       |
| (1,2509) | 1:211:A:LEU:HD21 | 1:211:A:LEU:HA   | 3                   | 0.27     | 0.02                | 0.26       |
| (1,2509) | 1:211:A:LEU:HD22 | 1:211:A:LEU:HA   | 3                   | 0.27     | 0.02                | 0.26       |
| (1,2509) | 1:211:A:LEU:HD23 | 1:211:A:LEU:HA   | 3                   | 0.27     | 0.02                | 0.26       |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD11 | 3                   | 0.26     | 0.05                | 0.24       |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD12 | 3                   | 0.26     | 0.05                | 0.24       |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD13 | 3                   | 0.26     | 0.05                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG11 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG12 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG13 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG11 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG12 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG13 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG11 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG12 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,190)  | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG13 | 3                   | 0.25     | 0.04                | 0.24       |
| (1,690)  | 2:686:B:ARG:HG3  | 2:686:B:ARG:H    | 3                   | 0.24     | 0.08                | 0.19       |
| (1,690)  | 2:685:B:LEU:HG   | 2:686:B:ARG:H    | 3                   | 0.24     | 0.08                | 0.19       |
| (1,1759) | 2:697:B:LEU:HD21 | 2:638:B:GLN:HE22 | 3                   | 0.24     | 0.05                | 0.27       |
| (1,1759) | 2:697:B:LEU:HD22 | 2:638:B:GLN:HE22 | 3                   | 0.24     | 0.05                | 0.27       |
| (1,1759) | 2:697:B:LEU:HD23 | 2:638:B:GLN:HE22 | 3                   | 0.24     | 0.05                | 0.27       |
| (1,1759) | 2:697:B:LEU:HD11 | 2:638:B:GLN:HE22 | 3                   | 0.24     | 0.05                | 0.27       |
| (1,1759) | 2:697:B:LEU:HD12 | 2:638:B:GLN:HE22 | 3                   | 0.24     | 0.05                | 0.27       |
| (1,1759) | 2:697:B:LEU:HD13 | 2:638:B:GLN:HE22 | 3                   | 0.24     | 0.05                | 0.27       |
| (1,668)  | 2:716:B:LYS:HA   | 2:718:B:TRP:H    | 3                   | 0.2      | 0.07                | 0.2        |
| (1,296)  | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB1  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB2  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB3  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB1  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB2  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB3  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB1  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB2  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB3  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD11 | 2:629:B:ALA:HB1  | 3                   | 0.2      | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,296)  | 2:665:B:ILE:HD11 | 2:629:B:ALA:HB2  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD11 | 2:629:B:ALA:HB3  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD12 | 2:629:B:ALA:HB1  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD12 | 2:629:B:ALA:HB2  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD12 | 2:629:B:ALA:HB3  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD13 | 2:629:B:ALA:HB1  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD13 | 2:629:B:ALA:HB2  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,296)  | 2:665:B:ILE:HD13 | 2:629:B:ALA:HB3  | 3                   | 0.2      | 0.04                | 0.18       |
| (1,13)   | 2:682:B:ILE:HG21 | 2:686:B:ARG:HD3  | 3                   | 0.2      | 0.09                | 0.15       |
| (1,13)   | 2:682:B:ILE:HG22 | 2:686:B:ARG:HD3  | 3                   | 0.2      | 0.09                | 0.15       |
| (1,13)   | 2:682:B:ILE:HG23 | 2:686:B:ARG:HD3  | 3                   | 0.2      | 0.09                | 0.15       |
| (1,1549) | 2:672:B:ARG:HG2  | 2:672:B:ARG:HA   | 3                   | 0.19     | 0.03                | 0.18       |
| (1,1539) | 2:702:B:MET:HB3  | 2:699:B:ARG:HA   | 3                   | 0.19     | 0.06                | 0.22       |
| (1,349)  | 2:687:B:LYS:HD2  | 2:687:B:LYS:HA   | 3                   | 0.17     | 0.02                | 0.17       |
| (1,38)   | 2:682:B:ILE:HA   | 2:696:B:VAL:HG11 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,38)   | 2:682:B:ILE:HA   | 2:696:B:VAL:HG12 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,38)   | 2:682:B:ILE:HA   | 2:696:B:VAL:HG13 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,534)  | 2:615:B:ASP:HB2  | 2:615:B:ASP:H    | 3                   | 0.16     | 0.04                | 0.15       |
| (1,534)  | 2:655:B:ASP:HB2  | 2:655:B:ASP:H    | 3                   | 0.16     | 0.04                | 0.15       |
| (1,2027) | 2:701:B:LYS:HE2  | 2:701:B:LYS:H    | 3                   | 0.15     | 0.02                | 0.14       |
| (1,1904) | 2:615:B:ASP:HA   | 2:616:B:GLU:H    | 3                   | 0.15     | 0.04                | 0.13       |
| (1,1920) | 2:725:B:TYR:HB2  | 2:725:B:TYR:H    | 3                   | 0.14     | 0.02                | 0.15       |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD11 | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD12 | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD13 | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG21 | 2                   | 2.0      | 0.43                | 2.0        |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG22 | 2                   | 2.0      | 0.43                | 2.0        |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG23 | 2                   | 2.0      | 0.43                | 2.0        |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG11 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG12 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG13 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG11 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG12 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG13 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG11 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG12 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG13 | 2                   | 1.26     | 0.04                | 1.26       |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG11 | 2                   | 1.12     | 0.01                | 1.12       |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG12 | 2                   | 1.12     | 0.01                | 1.12       |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG13 | 2                   | 1.12     | 0.01                | 1.12       |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG11 | 2                   | 1.0      | 0.1                 | 1.0        |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG12 | 2                   | 1.0      | 0.1                 | 1.0        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG13 | 2                   | 1.0      | 0.1                 | 1.0        |
| (1,599)  | 2:634:B:LEU:HD21 | 2:637:B:ILE:H    | 2                   | 0.86     | 0.25                | 0.86       |
| (1,599)  | 2:634:B:LEU:HD22 | 2:637:B:ILE:H    | 2                   | 0.86     | 0.25                | 0.86       |
| (1,599)  | 2:634:B:LEU:HD23 | 2:637:B:ILE:H    | 2                   | 0.86     | 0.25                | 0.86       |
| (1,537)  | 2:613:B:CYS:HB3  | 2:616:B:GLU:H    | 2                   | 0.84     | 0.12                | 0.84       |
| (1,537)  | 2:613:B:CYS:HB2  | 2:616:B:GLU:H    | 2                   | 0.84     | 0.12                | 0.84       |
| (1,2648) | 1:225:A:LYS:HG3  | 1:224:A:ASN:HA   | 2                   | 0.84     | 0.1                 | 0.84       |
| (1,627)  | 2:644:B:LEU:HB3  | 2:649:B:GLN:H    | 2                   | 0.82     | 0.66                | 0.82       |
| (1,627)  | 2:647:B:GLU:HB2  | 2:649:B:GLN:H    | 2                   | 0.82     | 0.66                | 0.82       |
| (1,144)  | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD11 | 2                   | 0.72     | 0.56                | 0.72       |
| (1,144)  | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD12 | 2                   | 0.72     | 0.56                | 0.72       |
| (1,144)  | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD13 | 2                   | 0.72     | 0.56                | 0.72       |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG21 | 2                   | 0.69     | 0.07                | 0.69       |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG22 | 2                   | 0.69     | 0.07                | 0.69       |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG23 | 2                   | 0.69     | 0.07                | 0.69       |
| (1,1992) | 2:633:B:VAL:HG11 | 2:633:B:VAL:H    | 2                   | 0.68     | 0.0                 | 0.68       |
| (1,1992) | 2:633:B:VAL:HG12 | 2:633:B:VAL:H    | 2                   | 0.68     | 0.0                 | 0.68       |
| (1,1992) | 2:633:B:VAL:HG13 | 2:633:B:VAL:H    | 2                   | 0.68     | 0.0                 | 0.68       |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD21 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD22 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD23 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD21 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD22 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD23 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD21 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD22 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD23 | 2                   | 0.68     | 0.34                | 0.68       |
| (1,436)  | 1:211:A:LEU:HA   | 2:703:B:LYS:HE2  | 2                   | 0.66     | 0.06                | 0.66       |
| (1,1599) | 2:668:B:LYS:HG2  | 2:668:B:LYS:HE2  | 2                   | 0.6      | 0.08                | 0.6        |
| (1,1631) | 1:211:A:LEU:HD11 | 2:703:B:LYS:HE2  | 2                   | 0.6      | 0.04                | 0.6        |
| (1,1631) | 1:211:A:LEU:HD12 | 2:703:B:LYS:HE2  | 2                   | 0.6      | 0.04                | 0.6        |
| (1,1631) | 1:211:A:LEU:HD13 | 2:703:B:LYS:HE2  | 2                   | 0.6      | 0.04                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD11 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD12 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD13 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD11 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD12 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD13 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD11 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD12 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD13 | 2                   | 0.6      | 0.09                | 0.6        |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG11 | 2                   | 0.58     | 0.04                | 0.58       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG12 | 2                   | 0.58     | 0.04                | 0.58       |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG13 | 2                   | 0.58     | 0.04                | 0.58       |
| (1,206)  | 2:686:B:ARG:HG2  | 2:653:B:ARG:HG2  | 2                   | 0.57     | 0.05                | 0.57       |
| (1,2310) | 2:616:B:GLU:HB3  | 2:616:B:GLU:H    | 2                   | 0.54     | 0.02                | 0.54       |
| (1,1713) | 2:686:B:ARG:HD3  | 2:683:B:ASP:HA   | 2                   | 0.52     | 0.15                | 0.52       |
| (1,899)  | 2:620:B:LEU:HA   | 2:623:B:VAL:HG11 | 2                   | 0.46     | 0.18                | 0.46       |
| (1,899)  | 2:620:B:LEU:HA   | 2:623:B:VAL:HG12 | 2                   | 0.46     | 0.18                | 0.46       |
| (1,899)  | 2:620:B:LEU:HA   | 2:623:B:VAL:HG13 | 2                   | 0.46     | 0.18                | 0.46       |
| (1,272)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HB3  | 2                   | 0.46     | 0.02                | 0.46       |
| (1,272)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HB3  | 2                   | 0.46     | 0.02                | 0.46       |
| (1,272)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HB3  | 2                   | 0.46     | 0.02                | 0.46       |
| (1,297)  | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB1  | 2                   | 0.45     | 0.35                | 0.45       |
| (1,297)  | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB2  | 2                   | 0.45     | 0.35                | 0.45       |
| (1,297)  | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB3  | 2                   | 0.45     | 0.35                | 0.45       |
| (1,298)  | 1:207:A:LEU:HG   | 2:710:B:ALA:HB1  | 2                   | 0.44     | 0.18                | 0.44       |
| (1,298)  | 1:207:A:LEU:HG   | 2:710:B:ALA:HB2  | 2                   | 0.44     | 0.18                | 0.44       |
| (1,298)  | 1:207:A:LEU:HG   | 2:710:B:ALA:HB3  | 2                   | 0.44     | 0.18                | 0.44       |
| (1,684)  | 2:716:B:LYS:HD3  | 2:717:B:VAL:H    | 2                   | 0.44     | 0.12                | 0.44       |
| (1,408)  | 2:634:B:LEU:HD11 | 2:697:B:LEU:HA   | 2                   | 0.44     | 0.03                | 0.44       |
| (1,408)  | 2:634:B:LEU:HD12 | 2:697:B:LEU:HA   | 2                   | 0.44     | 0.03                | 0.44       |
| (1,408)  | 2:634:B:LEU:HD13 | 2:697:B:LEU:HA   | 2                   | 0.44     | 0.03                | 0.44       |
| (1,408)  | 2:697:B:LEU:HD21 | 2:697:B:LEU:HA   | 2                   | 0.44     | 0.03                | 0.44       |
| (1,408)  | 2:697:B:LEU:HD22 | 2:697:B:LEU:HA   | 2                   | 0.44     | 0.03                | 0.44       |
| (1,408)  | 2:697:B:LEU:HD23 | 2:697:B:LEU:HA   | 2                   | 0.44     | 0.03                | 0.44       |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD11 | 2                   | 0.42     | 0.04                | 0.42       |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD12 | 2                   | 0.42     | 0.04                | 0.42       |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD13 | 2                   | 0.42     | 0.04                | 0.42       |
| (1,95)   | 2:662:B:SER:HB3  | 2:665:B:ILE:HD11 | 2                   | 0.42     | 0.29                | 0.42       |
| (1,95)   | 2:662:B:SER:HB3  | 2:665:B:ILE:HD12 | 2                   | 0.42     | 0.29                | 0.42       |
| (1,95)   | 2:662:B:SER:HB3  | 2:665:B:ILE:HD13 | 2                   | 0.42     | 0.29                | 0.42       |
| (1,1680) | 2:708:B:ARG:HB3  | 2:708:B:ARG:HD2  | 2                   | 0.41     | 0.0                 | 0.41       |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG21 | 2                   | 0.4      | 0.01                | 0.4        |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG22 | 2                   | 0.4      | 0.01                | 0.4        |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG23 | 2                   | 0.4      | 0.01                | 0.4        |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG11 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG12 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG13 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG11 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG12 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG13 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG11 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG12 | 2                   | 0.38     | 0.04                | 0.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG13 | 2                   | 0.38     | 0.04                | 0.38       |
| (1,1823) | 2:708:B:ARG:HG3  | 2:708:B:ARG:H    | 2                   | 0.38     | 0.01                | 0.38       |
| (1,319)  | 2:687:B:LYS:HA   | 2:653:B:ARG:HD2  | 2                   | 0.38     | 0.24                | 0.38       |
| (1,2294) | 2:691:B:ILE:HG13 | 2:691:B:ILE:H    | 2                   | 0.37     | 0.02                | 0.37       |
| (1,183)  | 2:667:B:ARG:HG3  | 2:682:B:ILE:HG21 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,183)  | 2:667:B:ARG:HG3  | 2:682:B:ILE:HG22 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,183)  | 2:667:B:ARG:HG3  | 2:682:B:ILE:HG23 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,183)  | 2:685:B:LEU:HG   | 2:682:B:ILE:HG21 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,183)  | 2:685:B:LEU:HG   | 2:682:B:ILE:HG22 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,183)  | 2:685:B:LEU:HG   | 2:682:B:ILE:HG23 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,938)  | 2:720:B:GLU:HA   | 2:724:B:LYS:HG3  | 2                   | 0.34     | 0.12                | 0.34       |
| (1,402)  | 2:632:B:ARG:HG3  | 2:632:B:ARG:HD3  | 2                   | 0.34     | 0.18                | 0.34       |
| (1,402)  | 2:712:B:ARG:HB2  | 2:712:B:ARG:HD2  | 2                   | 0.34     | 0.18                | 0.34       |
| (1,1817) | 2:709:B:GLU:HB3  | 2:710:B:ALA:H    | 2                   | 0.32     | 0.05                | 0.32       |
| (1,1817) | 2:709:B:GLU:HB2  | 2:710:B:ALA:H    | 2                   | 0.32     | 0.05                | 0.32       |
| (1,528)  | 2:611:B:TYR:HB2  | 2:611:B:TYR:H    | 2                   | 0.32     | 0.16                | 0.32       |
| (1,281)  | 2:622:B:VAL:HG11 | 2:619:B:GLU:HG3  | 2                   | 0.31     | 0.17                | 0.31       |
| (1,281)  | 2:622:B:VAL:HG12 | 2:619:B:GLU:HG3  | 2                   | 0.31     | 0.17                | 0.31       |
| (1,281)  | 2:622:B:VAL:HG13 | 2:619:B:GLU:HG3  | 2                   | 0.31     | 0.17                | 0.31       |
| (1,1818) | 2:708:B:ARG:HB2  | 2:709:B:GLU:H    | 2                   | 0.3      | 0.04                | 0.3        |
| (1,1418) | 2:717:B:VAL:HG11 | 2:720:B:GLU:HG2  | 2                   | 0.29     | 0.17                | 0.29       |
| (1,1418) | 2:717:B:VAL:HG12 | 2:720:B:GLU:HG2  | 2                   | 0.29     | 0.17                | 0.29       |
| (1,1418) | 2:717:B:VAL:HG13 | 2:720:B:GLU:HG2  | 2                   | 0.29     | 0.17                | 0.29       |
| (1,2773) | 1:225:A:LYS:HG3  | 1:225:A:LYS:H    | 2                   | 0.29     | 0.06                | 0.29       |
| (1,2773) | 1:225:A:LYS:HG2  | 1:225:A:LYS:H    | 2                   | 0.29     | 0.06                | 0.29       |
| (1,1944) | 2:623:B:VAL:HG11 | 2:623:B:VAL:H    | 2                   | 0.28     | 0.01                | 0.28       |
| (1,1944) | 2:623:B:VAL:HG12 | 2:623:B:VAL:H    | 2                   | 0.28     | 0.01                | 0.28       |
| (1,1944) | 2:623:B:VAL:HG13 | 2:623:B:VAL:H    | 2                   | 0.28     | 0.01                | 0.28       |
| (1,997)  | 2:668:B:LYS:HA   | 2:668:B:LYS:HD2  | 2                   | 0.27     | 0.04                | 0.27       |
| (1,269)  | 2:717:B:VAL:HG21 | 2:720:B:GLU:HB2  | 2                   | 0.26     | 0.04                | 0.26       |
| (1,269)  | 2:717:B:VAL:HG22 | 2:720:B:GLU:HB2  | 2                   | 0.26     | 0.04                | 0.26       |
| (1,269)  | 2:717:B:VAL:HG23 | 2:720:B:GLU:HB2  | 2                   | 0.26     | 0.04                | 0.26       |
| (1,269)  | 2:633:B:VAL:HG21 | 2:632:B:ARG:HB3  | 2                   | 0.26     | 0.04                | 0.26       |
| (1,269)  | 2:633:B:VAL:HG22 | 2:632:B:ARG:HB3  | 2                   | 0.26     | 0.04                | 0.26       |
| (1,269)  | 2:633:B:VAL:HG23 | 2:632:B:ARG:HB3  | 2                   | 0.26     | 0.04                | 0.26       |
| (1,2079) | 2:649:B:GLN:HG3  | 2:649:B:GLN:H    | 2                   | 0.26     | 0.02                | 0.26       |
| (1,616)  | 2:643:B:ARG:HG3  | 2:643:B:ARG:H    | 2                   | 0.26     | 0.05                | 0.26       |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD11 | 2                   | 0.24     | 0.01                | 0.24       |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD12 | 2                   | 0.24     | 0.01                | 0.24       |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD13 | 2                   | 0.24     | 0.01                | 0.24       |
| (1,97)   | 2:657:B:THR:HB   | 2:637:B:ILE:HD11 | 2                   | 0.24     | 0.02                | 0.24       |
| (1,97)   | 2:657:B:THR:HB   | 2:637:B:ILE:HD12 | 2                   | 0.24     | 0.02                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,97)   | 2:657:B:THR:HB   | 2:637:B:ILE:HD13 | 2                   | 0.24     | 0.02                | 0.24       |
| (1,657)  | 1:211:A:LEU:HD11 | 2:673:B:ILE:H    | 2                   | 0.24     | 0.03                | 0.24       |
| (1,657)  | 1:211:A:LEU:HD12 | 2:673:B:ILE:H    | 2                   | 0.24     | 0.03                | 0.24       |
| (1,657)  | 1:211:A:LEU:HD13 | 2:673:B:ILE:H    | 2                   | 0.24     | 0.03                | 0.24       |
| (1,657)  | 2:670:B:LEU:HD21 | 2:673:B:ILE:H    | 2                   | 0.24     | 0.03                | 0.24       |
| (1,657)  | 2:670:B:LEU:HD22 | 2:673:B:ILE:H    | 2                   | 0.24     | 0.03                | 0.24       |
| (1,657)  | 2:670:B:LEU:HD23 | 2:673:B:ILE:H    | 2                   | 0.24     | 0.03                | 0.24       |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG21 | 2                   | 0.23     | 0.11                | 0.23       |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG22 | 2                   | 0.23     | 0.11                | 0.23       |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG23 | 2                   | 0.23     | 0.11                | 0.23       |
| (1,193)  | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG21 | 2                   | 0.23     | 0.01                | 0.23       |
| (1,193)  | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG22 | 2                   | 0.23     | 0.01                | 0.23       |
| (1,193)  | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG23 | 2                   | 0.23     | 0.01                | 0.23       |
| (1,193)  | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG21 | 2                   | 0.23     | 0.01                | 0.23       |
| (1,193)  | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG22 | 2                   | 0.23     | 0.01                | 0.23       |
| (1,193)  | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG23 | 2                   | 0.23     | 0.01                | 0.23       |
| (1,763)  | 2:675:B:ALA:HA   | 1:210:A:LEU:HD11 | 2                   | 0.22     | 0.12                | 0.22       |
| (1,763)  | 2:675:B:ALA:HA   | 1:210:A:LEU:HD12 | 2                   | 0.22     | 0.12                | 0.22       |
| (1,763)  | 2:675:B:ALA:HA   | 1:210:A:LEU:HD13 | 2                   | 0.22     | 0.12                | 0.22       |
| (1,763)  | 1:212:A:THR:HA   | 1:210:A:LEU:HD11 | 2                   | 0.22     | 0.12                | 0.22       |
| (1,763)  | 1:212:A:THR:HA   | 1:210:A:LEU:HD12 | 2                   | 0.22     | 0.12                | 0.22       |
| (1,763)  | 1:212:A:THR:HA   | 1:210:A:LEU:HD13 | 2                   | 0.22     | 0.12                | 0.22       |
| (1,1979) | 2:628:B:LEU:HD21 | 2:630:B:THR:H    | 2                   | 0.22     | 0.05                | 0.22       |
| (1,1979) | 2:628:B:LEU:HD22 | 2:630:B:THR:H    | 2                   | 0.22     | 0.05                | 0.22       |
| (1,1979) | 2:628:B:LEU:HD23 | 2:630:B:THR:H    | 2                   | 0.22     | 0.05                | 0.22       |
| (1,341)  | 2:635:B:GLU:HB3  | 2:635:B:GLU:HA   | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1623) | 2:622:B:VAL:HG21 | 2:619:B:GLU:HA   | 2                   | 0.2      | 0.05                | 0.2        |
| (1,1623) | 2:622:B:VAL:HG22 | 2:619:B:GLU:HA   | 2                   | 0.2      | 0.05                | 0.2        |
| (1,1623) | 2:622:B:VAL:HG23 | 2:619:B:GLU:HA   | 2                   | 0.2      | 0.05                | 0.2        |
| (1,2673) | 1:206:A:GLN:HG3  | 1:206:A:GLN:H    | 2                   | 0.2      | 0.03                | 0.2        |
| (1,1480) | 2:699:B:ARG:HD3  | 2:699:B:ARG:HA   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD21 | 2                   | 0.19     | 0.06                | 0.19       |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD22 | 2                   | 0.19     | 0.06                | 0.19       |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD23 | 2                   | 0.19     | 0.06                | 0.19       |
| (1,2071) | 2:649:B:GLN:HG3  | 2:648:B:GLU:H    | 2                   | 0.18     | 0.01                | 0.18       |
| (1,42)   | 2:697:B:LEU:HA   | 2:697:B:LEU:HD11 | 2                   | 0.18     | 0.02                | 0.18       |
| (1,42)   | 2:697:B:LEU:HA   | 2:697:B:LEU:HD12 | 2                   | 0.18     | 0.02                | 0.18       |
| (1,42)   | 2:697:B:LEU:HA   | 2:697:B:LEU:HD13 | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD11 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD12 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD13 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,1670) | 2:721:B:GLN:HB2  | 2:721:B:GLN:HG3  | 2                   | 0.18     | 0.03                | 0.18       |

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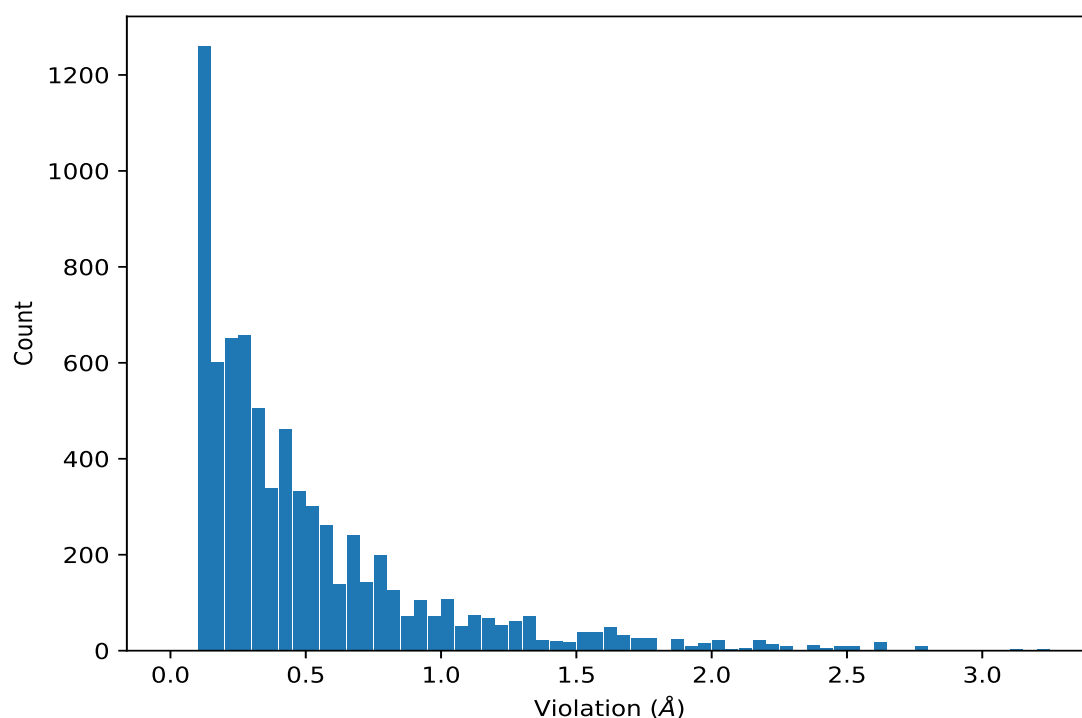
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1980) | 2:627:B:ASN:HD21 | 2:631:B:ILE:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,365)  | 2:712:B:ARG:HB2  | 2:712:B:ARG:HA   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2659) | 1:223:A:LEU:HA   | 1:226:A:LEU:HB2  | 2                   | 0.15     | 0.05                | 0.15       |
| (1,691)  | 2:654:B:LEU:HD21 | 2:686:B:ARG:H    | 2                   | 0.15     | 0.04                | 0.15       |
| (1,691)  | 2:654:B:LEU:HD22 | 2:686:B:ARG:H    | 2                   | 0.15     | 0.04                | 0.15       |
| (1,691)  | 2:654:B:LEU:HD23 | 2:686:B:ARG:H    | 2                   | 0.15     | 0.04                | 0.15       |
| (1,670)  | 2:674:B:TYR:HB3  | 2:678:B:ALA:H    | 2                   | 0.15     | 0.04                | 0.15       |
| (1,1600) | 2:648:B:GLU:HG3  | 2:651:B:LYS:HE3  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,1600) | 2:648:B:GLU:HG3  | 2:651:B:LYS:HE2  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,176)  | 2:700:B:LEU:HG   | 2:673:B:ILE:HD11 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,176)  | 2:700:B:LEU:HG   | 2:673:B:ILE:HD12 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,176)  | 2:700:B:LEU:HG   | 2:673:B:ILE:HD13 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,250)  | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB1  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,250)  | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB2  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,250)  | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB3  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,1415) | 2:687:B:LYS:HG3  | 2:687:B:LYS:HB2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1918) | 2:724:B:LYS:HA   | 2:725:B:TYR:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (1,2280) | 2:690:B:SER:HB2  | 2:690:B:SER:H    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,2704) | 1:212:A:THR:HG21 | 1:212:A:THR:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (1,2704) | 1:212:A:THR:HG22 | 1:212:A:THR:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (1,2704) | 1:212:A:THR:HG23 | 1:212:A:THR:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (2,2)    | 2:707:B:TRP:HD1  | 2:624:B:LEU:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1)    | 2:616:B:GLU:O    | 2:620:B:LEU:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,89)   | 2:714:B:PHE:O    | 2:718:B:TRP:H    | 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) |
|----------|------------------|------------------|----------|---------------|
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 16       | 3.25          |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 16       | 3.25          |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 16       | 3.25          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD21 | 13       | 3.13          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD22 | 13       | 3.13          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD23 | 13       | 3.13          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 14       | 2.79          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 2        | 2.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 2        | 2.62          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 2        | 2.62          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 2        | 2.62          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 2        | 2.62          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 2        | 2.62          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 2        | 2.62          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 2        | 2.62          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 2        | 2.62          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD21 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD22 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD23 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD21 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD22 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD23 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD21 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD22 | 13       | 2.62          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD23 | 13       | 2.62          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 10       | 2.51          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 8        | 2.46          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 8        | 2.46          |
| (1,1719) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE22 | 10       | 2.44          |
| (1,1719) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE22 | 10       | 2.44          |
| (1,1719) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE22 | 10       | 2.44          |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG21 | 7        | 2.43          |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG22 | 7        | 2.43          |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG23 | 7        | 2.43          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 2        | 2.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 2        | 2.4           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 2        | 2.4           |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 4        | 2.38          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 4        | 2.38          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD21 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD22 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD23 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD21 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD22 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD23 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD21 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD22 | 5        | 2.27          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD23 | 5        | 2.27          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 19       | 2.23          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 19       | 2.23          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 19       | 2.23          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 12       | 2.23          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD21 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD22 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD23 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD21 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD22 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD23 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD21 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD22 | 18       | 2.22          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD23 | 18       | 2.22          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 17       | 2.17          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 17       | 2.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 14       | 2.16          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 14       | 2.16          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 14       | 2.16          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 9        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 4        | 2.15          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 4        | 2.15          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 14       | 2.12          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 14       | 2.12          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 14       | 2.12          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 10       | 2.11          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 10       | 2.11          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 10       | 2.11          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 7        | 2.06          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 7        | 2.06          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 7        | 2.06          |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE2  | 16       | 2.05          |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE2  | 16       | 2.05          |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE2  | 16       | 2.05          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 4        | 2.03          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 4        | 2.03          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 4        | 2.03          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 5        | 2.02          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 5        | 2.02          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 5        | 2.02          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 5        | 2.02          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 5        | 2.02          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 5        | 2.02          |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD11 | 14       | 2.01          |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD12 | 14       | 2.01          |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD13 | 14       | 2.01          |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD11 | 14       | 2.01          |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD12 | 14       | 2.01          |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD13 | 14       | 2.01          |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD11 | 14       | 2.01          |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD12 | 14       | 2.01          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD13 | 14       | 2.01          |
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 20       | 1.98          |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 20       | 1.98          |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 20       | 1.98          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 12       | 1.98          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 12       | 1.98          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 12       | 1.98          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 7        | 1.97          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 7        | 1.97          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD21 | 2        | 1.93          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD22 | 2        | 1.93          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD23 | 2        | 1.93          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 5        | 1.93          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 5        | 1.93          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 5        | 1.93          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 5        | 1.93          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 5        | 1.93          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 5        | 1.93          |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD11 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD12 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD13 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD11 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD12 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD13 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD11 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD12 | 12       | 1.9           |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD13 | 12       | 1.9           |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 16       | 1.88          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 8        | 1.87          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 8        | 1.87          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 8        | 1.87          |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 5        | 1.87          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 3        | 1.85          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 3        | 1.85          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 3        | 1.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 3        | 1.85          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 3        | 1.85          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 3        | 1.85          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 3        | 1.85          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 3        | 1.85          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 3        | 1.85          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 16       | 1.79          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 16       | 1.79          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 16       | 1.79          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 16       | 1.79          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 16       | 1.79          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 16       | 1.79          |
| (1,1719) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE22 | 13       | 1.77          |
| (1,1719) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE22 | 13       | 1.77          |
| (1,1719) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE22 | 13       | 1.77          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 1        | 1.77          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 1        | 1.77          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 7        | 1.77          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 7        | 1.77          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 7        | 1.77          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 19       | 1.76          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 19       | 1.76          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 19       | 1.76          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 2        | 1.75          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 2        | 1.75          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 2        | 1.75          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 20       | 1.74          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 20       | 1.74          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 20       | 1.74          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 4        | 1.72          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 4        | 1.72          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 4        | 1.72          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 4        | 1.72          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 4        | 1.72          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 4        | 1.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 2        | 1.71          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 2        | 1.71          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD11 | 10       | 1.71          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD12 | 10       | 1.71          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD13 | 10       | 1.71          |
| (1,1122) | 2:716:B:LYS:HB2  | 2:717:B:VAL:HG11 | 8        | 1.71          |
| (1,1122) | 2:716:B:LYS:HB2  | 2:717:B:VAL:HG12 | 8        | 1.71          |
| (1,1122) | 2:716:B:LYS:HB2  | 2:717:B:VAL:HG13 | 8        | 1.71          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 11       | 1.71          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 11       | 1.71          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 11       | 1.71          |
| (1,2304) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE21 | 13       | 1.7           |
| (1,2304) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE21 | 13       | 1.7           |
| (1,2304) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE21 | 13       | 1.7           |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 13       | 1.69          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 13       | 1.69          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 13       | 1.69          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 6        | 1.68          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 6        | 1.68          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 6        | 1.68          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 2        | 1.68          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 2        | 1.68          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 2        | 1.68          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 16       | 1.67          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 16       | 1.67          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 16       | 1.67          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 16       | 1.67          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 16       | 1.67          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 16       | 1.67          |
| (1,765)  | 1:208:A:ASN:HB3  | 1:210:A:LEU:HD21 | 10       | 1.67          |
| (1,765)  | 1:208:A:ASN:HB3  | 1:210:A:LEU:HD22 | 10       | 1.67          |
| (1,765)  | 1:208:A:ASN:HB3  | 1:210:A:LEU:HD23 | 10       | 1.67          |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD11 | 5        | 1.66          |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD12 | 5        | 1.66          |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD13 | 5        | 1.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD11 | 5        | 1.66          |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD12 | 5        | 1.66          |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD13 | 5        | 1.66          |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD11 | 5        | 1.66          |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD12 | 5        | 1.66          |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD13 | 5        | 1.66          |
| (1,16)   | 2:624:B:LEU:HD21 | 2:708:B:ARG:HD2  | 7        | 1.66          |
| (1,16)   | 2:624:B:LEU:HD22 | 2:708:B:ARG:HD2  | 7        | 1.66          |
| (1,16)   | 2:624:B:LEU:HD23 | 2:708:B:ARG:HD2  | 7        | 1.66          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 16       | 1.65          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 16       | 1.65          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 8        | 1.65          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 8        | 1.65          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 8        | 1.65          |
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 9        | 1.64          |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 9        | 1.64          |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 9        | 1.64          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 9        | 1.64          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 9        | 1.64          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 9        | 1.64          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 5        | 1.63          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 5        | 1.63          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 5        | 1.63          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 18       | 1.63          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 18       | 1.63          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 18       | 1.63          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 4        | 1.62          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 4        | 1.62          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 4        | 1.62          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 4        | 1.62          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 4        | 1.62          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 4        | 1.62          |
| (1,213)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:HG3  | 6        | 1.62          |
| (1,213)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:HG3  | 6        | 1.62          |
| (1,213)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:HG3  | 6        | 1.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 20       | 1.62          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 20       | 1.62          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 20       | 1.62          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD21 | 2        | 1.61          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD22 | 2        | 1.61          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD23 | 2        | 1.61          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD11 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD12 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD13 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD11 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD12 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD13 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD11 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD12 | 4        | 1.6           |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD13 | 4        | 1.6           |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 14       | 1.59          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 14       | 1.59          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 14       | 1.59          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 11       | 1.58          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 11       | 1.58          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 11       | 1.58          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 11       | 1.58          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 11       | 1.58          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 11       | 1.58          |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG21 | 4        | 1.58          |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG22 | 4        | 1.58          |
| (1,1119) | 2:637:B:ILE:HG12 | 2:633:B:VAL:HG23 | 4        | 1.58          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 4        | 1.58          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 4        | 1.58          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 4        | 1.58          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 1        | 1.57          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 1        | 1.57          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 1        | 1.57          |
| (1,213)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:HG3  | 19       | 1.57          |
| (1,213)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:HG3  | 19       | 1.57          |
| (1,213)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:HG3  | 19       | 1.57          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD21 | 3        | 1.56          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD22 | 3        | 1.56          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD23 | 3        | 1.56          |
| (1,1719) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE22 | 6        | 1.56          |
| (1,1719) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE22 | 6        | 1.56          |
| (1,1719) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE22 | 6        | 1.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 6        | 1.56          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 6        | 1.56          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD21 | 3        | 1.55          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD22 | 3        | 1.55          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD23 | 3        | 1.55          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 3        | 1.54          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 3        | 1.54          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 3        | 1.54          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 14       | 1.53          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 14       | 1.53          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 14       | 1.53          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 14       | 1.53          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 14       | 1.53          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 14       | 1.53          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD11 | 7        | 1.53          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD12 | 7        | 1.53          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD13 | 7        | 1.53          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 14       | 1.52          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 14       | 1.52          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 14       | 1.52          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 14       | 1.52          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 14       | 1.52          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 14       | 1.52          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 14       | 1.52          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 14       | 1.52          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 13       | 1.52          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 13       | 1.52          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 13       | 1.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD11 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD12 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG21 | 2:670:B:LEU:HD13 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD11 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD12 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG22 | 2:670:B:LEU:HD13 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD11 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD12 | 17       | 1.5           |
| (1,434)  | 2:673:B:ILE:HG23 | 2:670:B:LEU:HD13 | 17       | 1.5           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 3        | 1.49          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 3        | 1.49          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 3        | 1.49          |
| (1,2590) | 2:677:B:LYS:HB2  | 1:220:A:LEU:HD11 | 9        | 1.48          |
| (1,2590) | 2:677:B:LYS:HB2  | 1:220:A:LEU:HD12 | 9        | 1.48          |
| (1,2590) | 2:677:B:LYS:HB2  | 1:220:A:LEU:HD13 | 9        | 1.48          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 2        | 1.48          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 2        | 1.48          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 2        | 1.48          |
| (1,627)  | 2:647:B:GLU:HB2  | 2:649:B:GLN:H    | 12       | 1.48          |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 6        | 1.48          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD11 | 3        | 1.48          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD12 | 3        | 1.48          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD13 | 3        | 1.48          |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 14       | 1.46          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 3        | 1.46          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 3        | 1.46          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 3        | 1.46          |
| (1,2304) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE21 | 7        | 1.44          |
| (1,2304) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE21 | 7        | 1.44          |
| (1,2304) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE21 | 7        | 1.44          |
| (1,463)  | 2:648:B:GLU:HA   | 2:649:B:GLN:HE22 | 14       | 1.44          |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 4        | 1.44          |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 1        | 1.43          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 7        | 1.42          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 7        | 1.42          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 7        | 1.42          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 11       | 1.42          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 11       | 1.42          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 11       | 1.42          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 11       | 1.42          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 11       | 1.42          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 11       | 1.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 20       | 1.42          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 15       | 1.41          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 15       | 1.41          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 15       | 1.41          |
| (1,463)  | 2:648:B:GLU:HA   | 2:649:B:GLN:HE22 | 2        | 1.39          |
| (1,237)  | 2:613:B:CYS:HB3  | 2:614:B:GLU:HG2  | 6        | 1.39          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 5        | 1.38          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 5        | 1.38          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 5        | 1.38          |
| (1,1489) | 2:653:B:ARG:HD2  | 2:687:B:LYS:HA   | 5        | 1.37          |
| (1,15)   | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD3  | 15       | 1.37          |
| (1,15)   | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD3  | 15       | 1.37          |
| (1,15)   | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD3  | 15       | 1.37          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD21 | 10       | 1.36          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD22 | 10       | 1.36          |
| (1,923)  | 2:693:B:VAL:HA   | 2:634:B:LEU:HD23 | 10       | 1.36          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 19       | 1.36          |
| (1,1719) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE22 | 7        | 1.35          |
| (1,1719) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE22 | 7        | 1.35          |
| (1,1719) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE22 | 7        | 1.35          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:640:B:LYS:HD3  | 18       | 1.35          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:640:B:LYS:HD3  | 18       | 1.35          |
| (1,271)  | 2:644:B:LEU:HD23 | 2:640:B:LYS:HD3  | 18       | 1.35          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD21 | 17       | 1.35          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD22 | 17       | 1.35          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD23 | 17       | 1.35          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD21 | 15       | 1.34          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD22 | 15       | 1.34          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD23 | 15       | 1.34          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 20       | 1.34          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 20       | 1.34          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 20       | 1.34          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 20       | 1.34          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 20       | 1.34          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 20       | 1.34          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD11 | 14       | 1.34          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD12 | 14       | 1.34          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD13 | 14       | 1.34          |
| (1,178)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:HD11 | 4        | 1.34          |
| (1,178)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:HD12 | 4        | 1.34          |
| (1,178)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:HD13 | 4        | 1.34          |
| (1,178)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:HD11 | 4        | 1.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,178)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:HD12 | 4        | 1.34          |
| (1,178)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:HD13 | 4        | 1.34          |
| (1,178)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:HD11 | 4        | 1.34          |
| (1,178)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:HD12 | 4        | 1.34          |
| (1,178)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:HD13 | 4        | 1.34          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 11       | 1.33          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 11       | 1.33          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 11       | 1.33          |
| (2,14)   | 1:220:A:LEU:HD21 | 1:217:A:MET:HG2  | 20       | 1.32          |
| (2,14)   | 1:220:A:LEU:HD22 | 1:217:A:MET:HG2  | 20       | 1.32          |
| (2,14)   | 1:220:A:LEU:HD23 | 1:217:A:MET:HG2  | 20       | 1.32          |
| (1,1716) | 1:211:A:LEU:HD21 | 2:703:B:LYS:HG2  | 13       | 1.32          |
| (1,1716) | 1:211:A:LEU:HD22 | 2:703:B:LYS:HG2  | 13       | 1.32          |
| (1,1716) | 1:211:A:LEU:HD23 | 2:703:B:LYS:HG2  | 13       | 1.32          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 10       | 1.32          |
| (1,656)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:H    | 6        | 1.32          |
| (1,656)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:H    | 6        | 1.32          |
| (1,656)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:H    | 6        | 1.32          |
| (1,213)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:HG3  | 10       | 1.32          |
| (1,213)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:HG3  | 10       | 1.32          |
| (1,213)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:HG3  | 10       | 1.32          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 18       | 1.31          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 18       | 1.31          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 18       | 1.31          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 14       | 1.31          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 14       | 1.31          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 14       | 1.31          |
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 15       | 1.3           |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 15       | 1.3           |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 15       | 1.3           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 10       | 1.3           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 10       | 1.3           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 10       | 1.3           |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 3        | 1.3           |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 3        | 1.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 13       | 1.3           |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 11       | 1.3           |
| (1,179)  | 2:697:B:LEU:HB3  | 2:631:B:ILE:HG21 | 16       | 1.3           |
| (1,179)  | 2:697:B:LEU:HB3  | 2:631:B:ILE:HG22 | 16       | 1.3           |
| (1,179)  | 2:697:B:LEU:HB3  | 2:631:B:ILE:HG23 | 16       | 1.3           |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG11 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG12 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG13 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG11 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG12 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG13 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG11 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG12 | 7        | 1.3           |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG13 | 7        | 1.3           |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 4        | 1.29          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 4        | 1.29          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 4        | 1.29          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 6        | 1.29          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 6        | 1.29          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 6        | 1.29          |
| (1,711)  | 2:670:B:LEU:HD21 | 2:675:B:ALA:H    | 17       | 1.29          |
| (1,711)  | 2:670:B:LEU:HD22 | 2:675:B:ALA:H    | 17       | 1.29          |
| (1,711)  | 2:670:B:LEU:HD23 | 2:675:B:ALA:H    | 17       | 1.29          |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 5        | 1.29          |
| (1,656)  | 2:670:B:LEU:HD11 | 2:673:B:ILE:H    | 4        | 1.28          |
| (1,656)  | 2:670:B:LEU:HD12 | 2:673:B:ILE:H    | 4        | 1.28          |
| (1,656)  | 2:670:B:LEU:HD13 | 2:673:B:ILE:H    | 4        | 1.28          |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 7        | 1.28          |
| (1,15)   | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD3  | 5        | 1.28          |
| (1,15)   | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD3  | 5        | 1.28          |
| (1,15)   | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD3  | 5        | 1.28          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 3        | 1.27          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 3        | 1.27          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 3        | 1.27          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 5        | 1.27          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 5        | 1.27          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 5        | 1.27          |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 15       | 1.27          |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 8        | 1.27          |
| (1,144)  | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD11 | 5        | 1.27          |
| (1,144)  | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD12 | 5        | 1.27          |
| (1,144)  | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD13 | 5        | 1.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 17       | 1.26          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 17       | 1.26          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 17       | 1.26          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD11 | 8        | 1.26          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD12 | 8        | 1.26          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD13 | 8        | 1.26          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD11 | 8        | 1.26          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD12 | 8        | 1.26          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD13 | 8        | 1.26          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 17       | 1.26          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 17       | 1.26          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 17       | 1.26          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 17       | 1.26          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 17       | 1.26          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 17       | 1.26          |
| (1,2304) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE21 | 6        | 1.25          |
| (1,2304) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE21 | 6        | 1.25          |
| (1,2304) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE21 | 6        | 1.25          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD11 | 17       | 1.25          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD12 | 17       | 1.25          |
| (1,1261) | 2:652:B:PHE:HD1  | 2:654:B:LEU:HD13 | 17       | 1.25          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD11 | 17       | 1.25          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD12 | 17       | 1.25          |
| (1,1261) | 2:652:B:PHE:HD2  | 2:654:B:LEU:HD13 | 17       | 1.25          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD11 | 20       | 1.25          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD12 | 20       | 1.25          |
| (1,1260) | 2:652:B:PHE:HE1  | 2:654:B:LEU:HD13 | 20       | 1.25          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD11 | 20       | 1.25          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD12 | 20       | 1.25          |
| (1,1260) | 2:652:B:PHE:HE2  | 2:654:B:LEU:HD13 | 20       | 1.25          |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 6        | 1.25          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD11 | 19       | 1.25          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD12 | 19       | 1.25          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD13 | 19       | 1.25          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 2        | 1.24          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 2        | 1.24          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 2        | 1.24          |
| (1,318)  | 2:655:B:ASP:HA   | 2:686:B:ARG:HD3  | 4        | 1.23          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD21 | 5        | 1.22          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD22 | 5        | 1.22          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD23 | 5        | 1.22          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD21 | 5        | 1.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD22 | 5        | 1.22          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD23 | 5        | 1.22          |
| (1,2304) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE21 | 10       | 1.22          |
| (1,2304) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE21 | 10       | 1.22          |
| (1,2304) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE21 | 10       | 1.22          |
| (1,855)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD3  | 10       | 1.22          |
| (1,855)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD3  | 10       | 1.22          |
| (1,855)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD3  | 10       | 1.22          |
| (1,658)  | 2:670:B:LEU:HD11 | 2:674:B:TYR:H    | 4        | 1.22          |
| (1,658)  | 2:670:B:LEU:HD12 | 2:674:B:TYR:H    | 4        | 1.22          |
| (1,658)  | 2:670:B:LEU:HD13 | 2:674:B:TYR:H    | 4        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 9        | 1.22          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 9        | 1.22          |
| (1,440)  | 2:697:B:LEU:HD21 | 2:638:B:GLN:HG3  | 12       | 1.22          |
| (1,440)  | 2:697:B:LEU:HD22 | 2:638:B:GLN:HG3  | 12       | 1.22          |
| (1,440)  | 2:697:B:LEU:HD23 | 2:638:B:GLN:HG3  | 12       | 1.22          |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG11 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG12 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB1  | 2:633:B:VAL:HG13 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG11 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG12 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB2  | 2:633:B:VAL:HG13 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG11 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG12 | 4        | 1.22          |
| (1,137)  | 2:629:B:ALA:HB3  | 2:633:B:VAL:HG13 | 4        | 1.22          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 8        | 1.21          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 8        | 1.21          |
| (1,855)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD3  | 14       | 1.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,855)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD3  | 14       | 1.21          |
| (1,855)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD3  | 14       | 1.21          |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 20       | 1.21          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 17       | 1.2           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 17       | 1.2           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 17       | 1.2           |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 14       | 1.2           |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 14       | 1.2           |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 14       | 1.2           |
| (1,433)  | 2:716:B:LYS:HB3  | 2:708:B:ARG:HD3  | 8        | 1.2           |
| (1,659)  | 2:670:B:LEU:HD21 | 2:674:B:TYR:H    | 2        | 1.19          |
| (1,659)  | 2:670:B:LEU:HD22 | 2:674:B:TYR:H    | 2        | 1.19          |
| (1,659)  | 2:670:B:LEU:HD23 | 2:674:B:TYR:H    | 2        | 1.19          |
| (1,440)  | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 14       | 1.19          |
| (1,440)  | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 14       | 1.19          |
| (1,440)  | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 14       | 1.19          |
| (1,432)  | 2:664:B:VAL:HB   | 2:668:B:LYS:HE2  | 17       | 1.19          |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD11 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD12 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD13 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD11 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD12 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD13 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD11 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD12 | 3        | 1.19          |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD13 | 3        | 1.19          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 13       | 1.19          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 13       | 1.19          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 13       | 1.19          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 1        | 1.18          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 1        | 1.18          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 1        | 1.18          |
| (1,2304) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE21 | 8        | 1.18          |
| (1,2304) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE21 | 8        | 1.18          |
| (1,2304) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE21 | 8        | 1.18          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 20       | 1.17          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 20       | 1.17          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 20       | 1.17          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 7        | 1.17          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 7        | 1.17          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 7        | 1.17          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 7        | 1.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 7        | 1.17          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 7        | 1.17          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 7        | 1.17          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 7        | 1.17          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 7        | 1.17          |
| (1,1489) | 2:653:B:ARG:HD2  | 2:687:B:LYS:HA   | 15       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 13       | 1.17          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 13       | 1.17          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 15       | 1.17          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 15       | 1.17          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 15       | 1.17          |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 3        | 1.17          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 6        | 1.16          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 6        | 1.16          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 6        | 1.16          |
| (1,658)  | 2:670:B:LEU:HD11 | 2:674:B:TYR:H    | 6        | 1.16          |
| (1,658)  | 2:670:B:LEU:HD12 | 2:674:B:TYR:H    | 6        | 1.16          |
| (1,658)  | 2:670:B:LEU:HD13 | 2:674:B:TYR:H    | 6        | 1.16          |
| (1,440)  | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 8        | 1.16          |
| (1,440)  | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 8        | 1.16          |
| (1,440)  | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 8        | 1.16          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 4        | 1.15          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 4        | 1.15          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 4        | 1.15          |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 5        | 1.15          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 18       | 1.14          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 18       | 1.14          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 18       | 1.14          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 11       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 20       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 20       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 20       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 20       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 20       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 20       | 1.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 20       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 20       | 1.14          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 20       | 1.14          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD11 | 13       | 1.14          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD12 | 13       | 1.14          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD13 | 13       | 1.14          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 12       | 1.13          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 12       | 1.13          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 12       | 1.13          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD21 | 8        | 1.13          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD22 | 8        | 1.13          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD23 | 8        | 1.13          |
| (1,456)  | 2:687:B:LYS:HD2  | 2:688:B:ASN:HD21 | 18       | 1.13          |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 7        | 1.13          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 4        | 1.13          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 14       | 1.12          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 14       | 1.12          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 14       | 1.12          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 10       | 1.12          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 10       | 1.12          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 10       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD21 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD22 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD11 | 2:644:B:LEU:HD23 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD21 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD22 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD12 | 2:644:B:LEU:HD23 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD21 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD22 | 11       | 1.12          |
| (1,445)  | 2:637:B:ILE:HD13 | 2:644:B:LEU:HD23 | 11       | 1.12          |
| (1,213)  | 2:628:B:LEU:HG   | 2:632:B:ARG:HG3  | 14       | 1.12          |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD11 | 12       | 1.12          |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD12 | 12       | 1.12          |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD13 | 12       | 1.12          |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG11 | 4        | 1.12          |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG12 | 4        | 1.12          |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG13 | 4        | 1.12          |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 4        | 1.11          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 12       | 1.11          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 12       | 1.11          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 12       | 1.11          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 19       | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG11 | 7        | 1.11          |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG12 | 7        | 1.11          |
| (1,33)   | 2:632:B:ARG:HA   | 2:633:B:VAL:HG13 | 7        | 1.11          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 5        | 1.1           |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 5        | 1.1           |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 5        | 1.1           |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 2        | 1.1           |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 20       | 1.1           |
| (1,658)  | 2:670:B:LEU:HD11 | 2:674:B:TYR:H    | 3        | 1.1           |
| (1,658)  | 2:670:B:LEU:HD12 | 2:674:B:TYR:H    | 3        | 1.1           |
| (1,658)  | 2:670:B:LEU:HD13 | 2:674:B:TYR:H    | 3        | 1.1           |
| (1,599)  | 2:634:B:LEU:HD21 | 2:637:B:ILE:H    | 7        | 1.1           |
| (1,599)  | 2:634:B:LEU:HD22 | 2:637:B:ILE:H    | 7        | 1.1           |
| (1,599)  | 2:634:B:LEU:HD23 | 2:637:B:ILE:H    | 7        | 1.1           |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 6        | 1.1           |
| (1,456)  | 1:223:A:LEU:HB3  | 2:688:B:ASN:HD21 | 11       | 1.1           |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 14       | 1.1           |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG11 | 16       | 1.09          |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG12 | 16       | 1.09          |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG13 | 16       | 1.09          |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 13       | 1.08          |
| (1,440)  | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 10       | 1.08          |
| (1,440)  | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 10       | 1.08          |
| (1,440)  | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 10       | 1.08          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG21 | 18       | 1.08          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG22 | 18       | 1.08          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG23 | 18       | 1.08          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 1        | 1.07          |
| (1,214)  | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 16       | 1.07          |
| (1,16)   | 2:664:B:VAL:HG21 | 2:667:B:ARG:HD3  | 15       | 1.07          |
| (1,16)   | 2:664:B:VAL:HG22 | 2:667:B:ARG:HD3  | 15       | 1.07          |
| (1,16)   | 2:664:B:VAL:HG23 | 2:667:B:ARG:HD3  | 15       | 1.07          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 6        | 1.06          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 6        | 1.06          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 6        | 1.06          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 19       | 1.06          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 19       | 1.06          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 19       | 1.06          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 7        | 1.06          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 4        | 1.06          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 4        | 1.06          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 4        | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD21 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD22 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD11 | 2:644:B:LEU:HD23 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD21 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD22 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD12 | 2:644:B:LEU:HD23 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD21 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD22 | 19       | 1.06          |
| (1,445)  | 2:654:B:LEU:HD13 | 2:644:B:LEU:HD23 | 19       | 1.06          |
| (1,440)  | 2:697:B:LEU:HD21 | 2:638:B:GLN:HG3  | 4        | 1.06          |
| (1,440)  | 2:697:B:LEU:HD22 | 2:638:B:GLN:HG3  | 4        | 1.06          |
| (1,440)  | 2:697:B:LEU:HD23 | 2:638:B:GLN:HG3  | 4        | 1.06          |
| (1,440)  | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 16       | 1.06          |
| (1,440)  | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 16       | 1.06          |
| (1,440)  | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 16       | 1.06          |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 4        | 1.06          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG21 | 19       | 1.06          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG22 | 19       | 1.06          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG23 | 19       | 1.06          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG11 | 18       | 1.05          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG12 | 18       | 1.05          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG13 | 18       | 1.05          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD21 | 13       | 1.05          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD22 | 13       | 1.05          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD23 | 13       | 1.05          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 8        | 1.05          |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 20       | 1.05          |
| (1,440)  | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 5        | 1.04          |
| (1,440)  | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 5        | 1.04          |
| (1,440)  | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 5        | 1.04          |
| (1,394)  | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE2  | 11       | 1.04          |
| (1,394)  | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE2  | 11       | 1.04          |
| (1,394)  | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE2  | 11       | 1.04          |
| (1,214)  | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 12       | 1.04          |
| (1,187)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HG11 | 5        | 1.04          |
| (1,187)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HG12 | 5        | 1.04          |
| (1,187)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HG13 | 5        | 1.04          |
| (1,187)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HG11 | 5        | 1.04          |
| (1,187)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HG12 | 5        | 1.04          |
| (1,187)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HG13 | 5        | 1.04          |
| (1,187)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HG11 | 5        | 1.04          |
| (1,187)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HG12 | 5        | 1.04          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,187)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HG13 | 5        | 1.04          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG21 | 15       | 1.04          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG22 | 15       | 1.04          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG23 | 15       | 1.04          |
| (1,74)   | 2:613:B:CYS:HB2  | 2:612:B:ARG:HB2  | 14       | 1.04          |
| (1,1740) | 2:691:B:ILE:HG12 | 2:688:B:ASN:HD22 | 7        | 1.03          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 6        | 1.03          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 13       | 1.03          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD2  | 6        | 1.03          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD2  | 6        | 1.03          |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD2  | 6        | 1.03          |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD21 | 11       | 1.03          |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD22 | 11       | 1.03          |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD23 | 11       | 1.03          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 7        | 1.02          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 7        | 1.02          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 7        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD21 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD22 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD23 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD21 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD22 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD23 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD21 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD22 | 5        | 1.02          |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD23 | 5        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD11 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD12 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD13 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD11 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD12 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD13 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD11 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD12 | 6        | 1.02          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD13 | 6        | 1.02          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 13       | 1.02          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 7        | 1.02          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 14       | 1.02          |
| (1,178)  | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD11 | 6        | 1.02          |
| (1,178)  | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD12 | 6        | 1.02          |
| (1,178)  | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD13 | 6        | 1.02          |
| (1,178)  | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD11 | 6        | 1.02          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,178)  | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD12 | 6        | 1.02          |
| (1,178)  | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD13 | 6        | 1.02          |
| (1,178)  | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD11 | 6        | 1.02          |
| (1,178)  | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD12 | 6        | 1.02          |
| (1,178)  | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD13 | 6        | 1.02          |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 3        | 1.01          |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 3        | 1.01          |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 3        | 1.01          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 2        | 1.01          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 2        | 1.01          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 2        | 1.01          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 17       | 1.01          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 17       | 1.01          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 17       | 1.01          |
| (1,855)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD3  | 7        | 1.01          |
| (1,855)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD3  | 7        | 1.01          |
| (1,855)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD3  | 7        | 1.01          |
| (1,756)  | 2:620:B:LEU:HD21 | 2:707:B:TRP:HE1  | 3        | 1.01          |
| (1,756)  | 2:620:B:LEU:HD22 | 2:707:B:TRP:HE1  | 3        | 1.01          |
| (1,756)  | 2:620:B:LEU:HD23 | 2:707:B:TRP:HE1  | 3        | 1.01          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 10       | 1.01          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG11 | 4        | 1.0           |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG12 | 4        | 1.0           |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG13 | 4        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD11 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD12 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD13 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD11 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD12 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD13 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD11 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD12 | 9        | 1.0           |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD13 | 9        | 1.0           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 1        | 1.0           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 1        | 1.0           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 1        | 1.0           |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 1        | 1.0           |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 1        | 1.0           |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 1        | 1.0           |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 16       | 1.0           |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG2  | 2        | 1.0           |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG2  | 2        | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG2  | 2        | 1.0           |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 3        | 1.0           |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 3        | 1.0           |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 3        | 1.0           |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 20       | 1.0           |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 20       | 1.0           |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 20       | 1.0           |
| (1,74)   | 2:613:B:CYS:HB2  | 2:612:B:ARG:HB2  | 4        | 1.0           |
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 14       | 0.99          |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 14       | 0.99          |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 14       | 0.99          |
| (1,1749) | 2:667:B:ARG:HD3  | 2:671:B:GLN:HE22 | 3        | 0.99          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 16       | 0.99          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 16       | 0.99          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 16       | 0.99          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 12       | 0.99          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 17       | 0.99          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 18       | 0.99          |
| (1,12)   | 2:718:B:TRP:HZ3  | 2:723:B:GLU:HA   | 14       | 0.99          |
| (2,18)   | 1:220:A:LEU:HD21 | 1:221:A:ARG:HG2  | 16       | 0.98          |
| (2,18)   | 1:220:A:LEU:HD22 | 1:221:A:ARG:HG2  | 16       | 0.98          |
| (2,18)   | 1:220:A:LEU:HD23 | 1:221:A:ARG:HG2  | 16       | 0.98          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 13       | 0.98          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 13       | 0.98          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 13       | 0.98          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 17       | 0.98          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 17       | 0.98          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 17       | 0.98          |
| (1,994)  | 2:705:B:GLU:HA   | 2:708:B:ARG:HB2  | 5        | 0.98          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 1        | 0.98          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE1  | 13       | 0.98          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE2  | 13       | 0.98          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE3  | 13       | 0.98          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 17       | 0.98          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD21 | 3        | 0.97          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD22 | 3        | 0.97          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD23 | 3        | 0.97          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD21 | 3        | 0.97          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD22 | 3        | 0.97          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD23 | 3        | 0.97          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 7        | 0.97          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 7        | 0.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 7        | 0.97          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 9        | 0.97          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 9        | 0.97          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 9        | 0.97          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD21 | 2        | 0.97          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD22 | 2        | 0.97          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD23 | 2        | 0.97          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 18       | 0.97          |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 15       | 0.97          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 15       | 0.97          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 15       | 0.97          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 15       | 0.97          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD3  | 20       | 0.97          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD3  | 20       | 0.97          |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD3  | 20       | 0.97          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD21 | 8        | 0.96          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD22 | 8        | 0.96          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD23 | 8        | 0.96          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD21 | 8        | 0.96          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD22 | 8        | 0.96          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD23 | 8        | 0.96          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 10       | 0.96          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 8        | 0.96          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 8        | 0.96          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 8        | 0.96          |
| (1,537)  | 2:613:B:CYS:HB2  | 2:616:B:GLU:H    | 6        | 0.96          |
| (1,440)  | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 6        | 0.96          |
| (1,440)  | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 6        | 0.96          |
| (1,440)  | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 6        | 0.96          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD3  | 14       | 0.96          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD3  | 14       | 0.96          |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD3  | 14       | 0.96          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 20       | 0.96          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 20       | 0.96          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 20       | 0.96          |
| (1,15)   | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD3  | 14       | 0.96          |
| (1,15)   | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD3  | 14       | 0.96          |
| (1,15)   | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD3  | 14       | 0.96          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 16       | 0.95          |
| (1,698)  | 1:223:A:LEU:HD11 | 2:688:B:ASN:H    | 10       | 0.95          |
| (1,698)  | 1:223:A:LEU:HD12 | 2:688:B:ASN:H    | 10       | 0.95          |
| (1,698)  | 1:223:A:LEU:HD13 | 2:688:B:ASN:H    | 10       | 0.95          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 3        | 0.95          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 4        | 0.95          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 4        | 0.95          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 4        | 0.95          |
| (1,214)  | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 1        | 0.95          |
| (1,2648) | 1:225:A:LYS:HG3  | 1:224:A:ASN:HA   | 6        | 0.94          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 1        | 0.94          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 1        | 0.94          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 1        | 0.94          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 5        | 0.94          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 5        | 0.94          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 5        | 0.94          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD11 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD12 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD13 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD11 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD12 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD13 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD11 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD12 | 13       | 0.94          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD13 | 13       | 0.94          |
| (1,863)  | 2:697:B:LEU:HD11 | 2:631:B:ILE:HA   | 8        | 0.94          |
| (1,863)  | 2:697:B:LEU:HD12 | 2:631:B:ILE:HA   | 8        | 0.94          |
| (1,863)  | 2:697:B:LEU:HD13 | 2:631:B:ILE:HA   | 8        | 0.94          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 20       | 0.94          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 11       | 0.94          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 11       | 0.94          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 11       | 0.94          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 4        | 0.94          |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 18       | 0.94          |
| (1,432)  | 2:700:B:LEU:HG   | 2:701:B:LYS:HE3  | 16       | 0.94          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 18       | 0.94          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 18       | 0.94          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 18       | 0.94          |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD11 | 6        | 0.94          |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD12 | 6        | 0.94          |
| (1,192)  | 2:685:B:LEU:HD21 | 2:670:B:LEU:HD13 | 6        | 0.94          |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD11 | 6        | 0.94          |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD12 | 6        | 0.94          |
| (1,192)  | 2:685:B:LEU:HD22 | 2:670:B:LEU:HD13 | 6        | 0.94          |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD11 | 6        | 0.94          |
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD12 | 6        | 0.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,192)  | 2:685:B:LEU:HD23 | 2:670:B:LEU:HD13 | 6        | 0.94          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 8        | 0.93          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 14       | 0.93          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 12       | 0.93          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 12       | 0.93          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 12       | 0.93          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 16       | 0.93          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 16       | 0.93          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 16       | 0.93          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 17       | 0.93          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 17       | 0.93          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 17       | 0.93          |
| (1,74)   | 2:613:B:CYS:HB3  | 2:612:B:ARG:HB2  | 1        | 0.93          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD21 | 13       | 0.92          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD22 | 13       | 0.92          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD23 | 13       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD11 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD12 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD13 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD11 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD12 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD13 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD11 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD12 | 20       | 0.92          |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD13 | 20       | 0.92          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 8        | 0.92          |
| (1,711)  | 2:670:B:LEU:HD21 | 2:675:B:ALA:H    | 3        | 0.92          |
| (1,711)  | 2:670:B:LEU:HD22 | 2:675:B:ALA:H    | 3        | 0.92          |
| (1,711)  | 2:670:B:LEU:HD23 | 2:675:B:ALA:H    | 3        | 0.92          |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 7        | 0.92          |
| (2,18)   | 1:220:A:LEU:HD21 | 1:221:A:ARG:HG2  | 20       | 0.91          |
| (2,18)   | 1:220:A:LEU:HD22 | 1:221:A:ARG:HG2  | 20       | 0.91          |
| (2,18)   | 1:220:A:LEU:HD23 | 1:221:A:ARG:HG2  | 20       | 0.91          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 5        | 0.91          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 5        | 0.91          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 5        | 0.91          |
| (1,238)  | 2:646:B:ALA:HB1  | 2:647:B:GLU:HG3  | 11       | 0.91          |
| (1,238)  | 2:646:B:ALA:HB2  | 2:647:B:GLU:HG3  | 11       | 0.91          |
| (1,238)  | 2:646:B:ALA:HB3  | 2:647:B:GLU:HG3  | 11       | 0.91          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 20       | 0.9           |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 20       | 0.9           |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 20       | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1413) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HG3  | 4        | 0.9           |
| (1,1413) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HG3  | 4        | 0.9           |
| (1,1413) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HG3  | 4        | 0.9           |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG11 | 5        | 0.9           |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG12 | 5        | 0.9           |
| (1,1124) | 2:619:B:GLU:HG2  | 2:623:B:VAL:HG13 | 5        | 0.9           |
| (1,711)  | 1:211:A:LEU:HD11 | 2:675:B:ALA:H    | 2        | 0.9           |
| (1,711)  | 1:211:A:LEU:HD12 | 2:675:B:ALA:H    | 2        | 0.9           |
| (1,711)  | 1:211:A:LEU:HD13 | 2:675:B:ALA:H    | 2        | 0.9           |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 10       | 0.9           |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 7        | 0.9           |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG21 | 11       | 0.9           |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG22 | 11       | 0.9           |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG23 | 11       | 0.9           |
| (1,129)  | 2:632:B:ARG:HG2  | 2:633:B:VAL:HG21 | 7        | 0.9           |
| (1,129)  | 2:632:B:ARG:HG2  | 2:633:B:VAL:HG22 | 7        | 0.9           |
| (1,129)  | 2:632:B:ARG:HG2  | 2:633:B:VAL:HG23 | 7        | 0.9           |
| (1,1908) | 2:617:B:ARG:HG3  | 2:616:B:GLU:H    | 3        | 0.89          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 13       | 0.89          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 13       | 0.89          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 14       | 0.89          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 14       | 0.89          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 14       | 0.89          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 15       | 0.89          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 12       | 0.89          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 12       | 0.89          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 12       | 0.89          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 14       | 0.89          |
| (1,74)   | 2:613:B:CYS:HB2  | 2:612:B:ARG:HB2  | 3        | 0.89          |
| (1,74)   | 2:613:B:CYS:HB2  | 2:612:B:ARG:HB2  | 10       | 0.89          |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD11 | 10       | 0.88          |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD12 | 10       | 0.88          |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD13 | 10       | 0.88          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 1        | 0.88          |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 1        | 0.88          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 1        | 0.88          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 5        | 0.88          |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 10       | 0.88          |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 5        | 0.88          |
| (1,391)  | 2:716:B:LYS:HB2  | 2:716:B:LYS:HE2  | 17       | 0.88          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 1        | 0.88          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 1        | 0.88          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 1        | 0.88          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 8        | 0.87          |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 8        | 0.87          |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 8        | 0.87          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 15       | 0.87          |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 15       | 0.87          |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 15       | 0.87          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD21 | 10       | 0.87          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD22 | 10       | 0.87          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD23 | 10       | 0.87          |
| (1,238)  | 2:646:B:ALA:HB1  | 2:647:B:GLU:HG2  | 8        | 0.87          |
| (1,238)  | 2:646:B:ALA:HB2  | 2:647:B:GLU:HG2  | 8        | 0.87          |
| (1,238)  | 2:646:B:ALA:HB3  | 2:647:B:GLU:HG2  | 8        | 0.87          |
| (1,214)  | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 14       | 0.87          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 5        | 0.87          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD3  | 1        | 0.87          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD3  | 1        | 0.87          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD3  | 1        | 0.87          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 5        | 0.86          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD11 | 3        | 0.86          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD12 | 3        | 0.86          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD13 | 3        | 0.86          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD11 | 3        | 0.86          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD12 | 3        | 0.86          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD13 | 3        | 0.86          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 7        | 0.86          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 7        | 0.86          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 7        | 0.86          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 9        | 0.86          |
| (1,463)  | 2:720:B:GLU:HA   | 2:721:B:GLN:HE22 | 7        | 0.86          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 19       | 0.86          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 19       | 0.86          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 19       | 0.86          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD3  | 9        | 0.86          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD3  | 9        | 0.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD3  | 9        | 0.86          |
| (1,266)  | 2:685:B:LEU:HD21 | 2:634:B:LEU:HG   | 15       | 0.86          |
| (1,266)  | 2:685:B:LEU:HD22 | 2:634:B:LEU:HG   | 15       | 0.86          |
| (1,266)  | 2:685:B:LEU:HD23 | 2:634:B:LEU:HG   | 15       | 0.86          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 9        | 0.85          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 14       | 0.85          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 13       | 0.85          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 16       | 0.85          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 16       | 0.85          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 16       | 0.85          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 10       | 0.85          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 10       | 0.85          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 10       | 0.85          |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG11 | 9        | 0.85          |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG12 | 9        | 0.85          |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG13 | 9        | 0.85          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 8        | 0.84          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 8        | 0.84          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 8        | 0.84          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 10       | 0.84          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 10       | 0.84          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 10       | 0.84          |
| (1,854)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD2  | 4        | 0.84          |
| (1,854)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD2  | 4        | 0.84          |
| (1,854)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD2  | 4        | 0.84          |
| (1,761)  | 2:713:B:GLY:HA3  | 1:207:A:LEU:HD21 | 3        | 0.84          |
| (1,761)  | 2:713:B:GLY:HA3  | 1:207:A:LEU:HD22 | 3        | 0.84          |
| (1,761)  | 2:713:B:GLY:HA3  | 1:207:A:LEU:HD23 | 3        | 0.84          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 17       | 0.84          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 17       | 0.84          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 17       | 0.84          |
| (1,391)  | 2:728:B:LYS:HB3  | 2:728:B:LYS:HE2  | 13       | 0.84          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD21 | 18       | 0.84          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD22 | 18       | 0.84          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD23 | 18       | 0.84          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 9        | 0.83          |
| (1,854)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD2  | 20       | 0.83          |
| (1,854)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD2  | 20       | 0.83          |
| (1,854)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD2  | 20       | 0.83          |
| (1,442)  | 2:644:B:LEU:HD21 | 2:649:B:GLN:HG3  | 19       | 0.83          |
| (1,442)  | 2:644:B:LEU:HD22 | 2:649:B:GLN:HG3  | 19       | 0.83          |
| (1,442)  | 2:644:B:LEU:HD23 | 2:649:B:GLN:HG3  | 19       | 0.83          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,391)  | 2:716:B:LYS:HB2  | 2:716:B:LYS:HE2  | 9        | 0.83          |
| (1,391)  | 2:728:B:LYS:HB3  | 2:728:B:LYS:HE3  | 11       | 0.83          |
| (1,279)  | 2:697:B:LEU:HD11 | 2:638:B:GLN:HG3  | 3        | 0.83          |
| (1,279)  | 2:697:B:LEU:HD12 | 2:638:B:GLN:HG3  | 3        | 0.83          |
| (1,279)  | 2:697:B:LEU:HD13 | 2:638:B:GLN:HG3  | 3        | 0.83          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD21 | 3        | 0.82          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD22 | 3        | 0.82          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD23 | 3        | 0.82          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 2        | 0.82          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 16       | 0.82          |
| (1,1852) | 2:701:B:LYS:HD2  | 2:700:B:LEU:H    | 10       | 0.82          |
| (1,1719) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE22 | 8        | 0.82          |
| (1,1719) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE22 | 8        | 0.82          |
| (1,1719) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE22 | 8        | 0.82          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 7        | 0.82          |
| (1,854)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD2  | 8        | 0.82          |
| (1,854)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD2  | 8        | 0.82          |
| (1,854)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD2  | 8        | 0.82          |
| (1,854)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD2  | 12       | 0.82          |
| (1,854)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD2  | 12       | 0.82          |
| (1,854)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD2  | 12       | 0.82          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD21 | 11       | 0.82          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD22 | 11       | 0.82          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD23 | 11       | 0.82          |
| (1,391)  | 2:728:B:LYS:HB3  | 2:728:B:LYS:HE2  | 1        | 0.82          |
| (1,266)  | 2:658:B:LEU:HD11 | 2:634:B:LEU:HG   | 12       | 0.82          |
| (1,266)  | 2:658:B:LEU:HD12 | 2:634:B:LEU:HG   | 12       | 0.82          |
| (1,266)  | 2:658:B:LEU:HD13 | 2:634:B:LEU:HG   | 12       | 0.82          |
| (1,2197) | 2:677:B:LYS:HE3  | 2:677:B:LYS:H    | 20       | 0.81          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 10       | 0.81          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 16       | 0.81          |
| (1,854)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD2  | 13       | 0.81          |
| (1,854)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD2  | 13       | 0.81          |
| (1,854)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD2  | 13       | 0.81          |
| (1,854)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HD2  | 16       | 0.81          |
| (1,854)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HD2  | 16       | 0.81          |
| (1,854)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HD2  | 16       | 0.81          |
| (1,456)  | 2:687:B:LYS:HD2  | 2:688:B:ASN:HD21 | 6        | 0.81          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD21 | 15       | 0.81          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD22 | 15       | 0.81          |
| (1,445)  | 2:654:B:LEU:HD21 | 2:644:B:LEU:HD23 | 15       | 0.81          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD21 | 15       | 0.81          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD22 | 15       | 0.81          |
| (1,445)  | 2:654:B:LEU:HD22 | 2:644:B:LEU:HD23 | 15       | 0.81          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD21 | 15       | 0.81          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD22 | 15       | 0.81          |
| (1,445)  | 2:654:B:LEU:HD23 | 2:644:B:LEU:HD23 | 15       | 0.81          |
| (1,391)  | 2:716:B:LYS:HB3  | 2:716:B:LYS:HE3  | 20       | 0.81          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 2        | 0.81          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 2        | 0.81          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 2        | 0.81          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 14       | 0.81          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 14       | 0.81          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 14       | 0.81          |
| (1,16)   | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD3  | 9        | 0.81          |
| (1,16)   | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD3  | 9        | 0.81          |
| (1,16)   | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD3  | 9        | 0.81          |
| (1,15)   | 2:631:B:ILE:HG21 | 2:632:B:ARG:HD2  | 12       | 0.81          |
| (1,15)   | 2:631:B:ILE:HG22 | 2:632:B:ARG:HD2  | 12       | 0.81          |
| (1,15)   | 2:631:B:ILE:HG23 | 2:632:B:ARG:HD2  | 12       | 0.81          |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD11 | 19       | 0.8           |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD12 | 19       | 0.8           |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD13 | 19       | 0.8           |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD21 | 2        | 0.8           |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD22 | 2        | 0.8           |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD23 | 2        | 0.8           |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 7        | 0.8           |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 7        | 0.8           |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 7        | 0.8           |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 7        | 0.8           |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 11       | 0.8           |
| (1,1489) | 2:653:B:ARG:HD2  | 2:687:B:LYS:HA   | 7        | 0.8           |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 16       | 0.8           |
| (1,659)  | 2:670:B:LEU:HD21 | 2:674:B:TYR:H    | 13       | 0.8           |
| (1,659)  | 2:670:B:LEU:HD22 | 2:674:B:TYR:H    | 13       | 0.8           |
| (1,659)  | 2:670:B:LEU:HD23 | 2:674:B:TYR:H    | 13       | 0.8           |
| (1,315)  | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 3        | 0.8           |
| (1,297)  | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB1  | 7        | 0.8           |
| (1,297)  | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB2  | 7        | 0.8           |
| (1,297)  | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB3  | 7        | 0.8           |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 1        | 0.8           |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 1        | 0.8           |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 1        | 0.8           |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG2  | 19       | 0.8           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG2  | 19       | 0.8           |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG2  | 19       | 0.8           |
| (1,238)  | 2:716:B:LYS:HG3  | 2:720:B:GLU:HG3  | 12       | 0.8           |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 6        | 0.8           |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 4        | 0.79          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 4        | 0.79          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 4        | 0.79          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 8        | 0.79          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 8        | 0.79          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 8        | 0.79          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 13       | 0.79          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 2        | 0.79          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 19       | 0.79          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 19       | 0.79          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 19       | 0.79          |
| (1,317)  | 2:712:B:ARG:HA   | 2:712:B:ARG:HD2  | 13       | 0.79          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 5        | 0.79          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 5        | 0.79          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 5        | 0.79          |
| (1,237)  | 2:613:B:CYS:HB2  | 2:616:B:GLU:HG3  | 11       | 0.79          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 10       | 0.79          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD11 | 2        | 0.79          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD12 | 2        | 0.79          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD13 | 2        | 0.79          |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 15       | 0.78          |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 15       | 0.78          |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 15       | 0.78          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 5        | 0.78          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 5        | 0.78          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 5        | 0.78          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 11       | 0.78          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 11       | 0.78          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 11       | 0.78          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 18       | 0.78          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 18       | 0.78          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 18       | 0.78          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 1        | 0.78          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 12       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 17       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 17       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 17       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 17       | 0.78          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 17       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 17       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 17       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 17       | 0.78          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 17       | 0.78          |
| (1,1682) | 2:606:B:ASN:HB2  | 2:610:B:ILE:HG13 | 1        | 0.78          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 14       | 0.78          |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD11 | 7        | 0.78          |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD12 | 7        | 0.78          |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD13 | 7        | 0.78          |
| (1,750)  | 2:670:B:LEU:HB2  | 2:672:B:ARG:H    | 6        | 0.78          |
| (1,711)  | 1:211:A:LEU:HD11 | 2:675:B:ALA:H    | 13       | 0.78          |
| (1,711)  | 1:211:A:LEU:HD12 | 2:675:B:ALA:H    | 13       | 0.78          |
| (1,711)  | 1:211:A:LEU:HD13 | 2:675:B:ALA:H    | 13       | 0.78          |
| (1,456)  | 2:687:B:LYS:HD2  | 2:688:B:ASN:HD21 | 13       | 0.78          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 5        | 0.78          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 5        | 0.78          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 5        | 0.78          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 20       | 0.78          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 20       | 0.78          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 20       | 0.78          |
| (1,391)  | 2:728:B:LYS:HB3  | 2:728:B:LYS:HE3  | 2        | 0.78          |
| (1,373)  | 2:721:B:GLN:HB2  | 2:718:B:TRP:HA   | 10       | 0.78          |
| (1,316)  | 2:716:B:LYS:HA   | 2:719:B:ARG:HD3  | 17       | 0.78          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 13       | 0.78          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 13       | 0.78          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 13       | 0.78          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 17       | 0.78          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 17       | 0.78          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 17       | 0.78          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 11       | 0.77          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 1        | 0.77          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 1        | 0.77          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 17       | 0.77          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 17       | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 17       | 0.77          |
| (1,761)  | 2:620:B:LEU:HA   | 1:207:A:LEU:HD21 | 4        | 0.77          |
| (1,761)  | 2:620:B:LEU:HA   | 1:207:A:LEU:HD22 | 4        | 0.77          |
| (1,761)  | 2:620:B:LEU:HA   | 1:207:A:LEU:HD23 | 4        | 0.77          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 9        | 0.77          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 2        | 0.77          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 2        | 0.77          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 2        | 0.77          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 7        | 0.77          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 7        | 0.77          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 7        | 0.77          |
| (1,279)  | 2:624:B:LEU:HD21 | 2:711:B:GLN:HG2  | 9        | 0.77          |
| (1,279)  | 2:624:B:LEU:HD22 | 2:711:B:GLN:HG2  | 9        | 0.77          |
| (1,279)  | 2:624:B:LEU:HD23 | 2:711:B:GLN:HG2  | 9        | 0.77          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD2  | 5        | 0.77          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD2  | 5        | 0.77          |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD2  | 5        | 0.77          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD3  | 8        | 0.77          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD3  | 8        | 0.77          |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD3  | 8        | 0.77          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 18       | 0.77          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 18       | 0.77          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 18       | 0.77          |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD21 | 13       | 0.77          |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD22 | 13       | 0.77          |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD23 | 13       | 0.77          |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD2  | 15       | 0.77          |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG21 | 5        | 0.76          |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG22 | 5        | 0.76          |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG23 | 5        | 0.76          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 2        | 0.76          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 2        | 0.76          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 2        | 0.76          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 14       | 0.76          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 14       | 0.76          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 14       | 0.76          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 20       | 0.76          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 20       | 0.76          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 20       | 0.76          |
| (1,1908) | 2:617:B:ARG:HG3  | 2:616:B:GLU:H    | 19       | 0.76          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 20       | 0.76          |
| (1,1489) | 2:653:B:ARG:HD2  | 2:687:B:LYS:HA   | 13       | 0.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 6        | 0.76          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 6        | 0.76          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 5        | 0.76          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 5        | 0.76          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 5        | 0.76          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 13       | 0.76          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 13       | 0.76          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 13       | 0.76          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 5        | 0.76          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 5        | 0.76          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 5        | 0.76          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 20       | 0.76          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 20       | 0.76          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 20       | 0.76          |
| (1,750)  | 2:670:B:LEU:HB2  | 2:672:B:ARG:H    | 3        | 0.76          |
| (1,750)  | 2:670:B:LEU:HB2  | 2:672:B:ARG:H    | 4        | 0.76          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 12       | 0.76          |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 19       | 0.76          |
| (1,389)  | 2:677:B:LYS:HG2  | 2:677:B:LYS:HE2  | 16       | 0.76          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB2  | 6        | 0.76          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB2  | 6        | 0.76          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB2  | 6        | 0.76          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 20       | 0.76          |
| (1,155)  | 2:638:B:GLN:HB3  | 2:641:B:LEU:HD11 | 19       | 0.76          |
| (1,155)  | 2:638:B:GLN:HB3  | 2:641:B:LEU:HD12 | 19       | 0.76          |
| (1,155)  | 2:638:B:GLN:HB3  | 2:641:B:LEU:HD13 | 19       | 0.76          |
| (1,16)   | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD2  | 12       | 0.76          |
| (1,16)   | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD2  | 12       | 0.76          |
| (1,16)   | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD2  | 12       | 0.76          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 14       | 0.75          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 14       | 0.75          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 14       | 0.75          |
| (1,2136) | 2:696:B:VAL:HG21 | 2:696:B:VAL:H    | 17       | 0.75          |
| (1,2136) | 2:696:B:VAL:HG22 | 2:696:B:VAL:H    | 17       | 0.75          |
| (1,2136) | 2:696:B:VAL:HG23 | 2:696:B:VAL:H    | 17       | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1852) | 2:701:B:LYS:HD2  | 2:700:B:LEU:H    | 17       | 0.75          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 11       | 0.75          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 11       | 0.75          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 11       | 0.75          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 14       | 0.75          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 14       | 0.75          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 14       | 0.75          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD11 | 6        | 0.75          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD12 | 6        | 0.75          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD13 | 6        | 0.75          |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 3        | 0.75          |
| (1,456)  | 1:226:A:LEU:HB3  | 2:688:B:ASN:HD21 | 4        | 0.75          |
| (1,429)  | 2:640:B:LYS:HA   | 2:640:B:LYS:HD3  | 17       | 0.75          |
| (1,391)  | 2:716:B:LYS:HB2  | 2:716:B:LYS:HE2  | 7        | 0.75          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 11       | 0.75          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 11       | 0.75          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 11       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 10       | 0.75          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 10       | 0.75          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 5        | 0.75          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 5        | 0.75          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 16       | 0.74          |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 16       | 0.74          |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 16       | 0.74          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 6        | 0.74          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 6        | 0.74          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 6        | 0.74          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 14       | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1908) | 2:617:B:ARG:HG3  | 2:616:B:GLU:H    | 15       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 17       | 0.74          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 17       | 0.74          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 10       | 0.74          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 10       | 0.74          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 10       | 0.74          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD11 | 14       | 0.74          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD12 | 14       | 0.74          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD13 | 14       | 0.74          |
| (1,456)  | 2:687:B:LYS:HD2  | 2:688:B:ASN:HD21 | 15       | 0.74          |
| (1,317)  | 2:712:B:ARG:HA   | 2:712:B:ARG:HD2  | 20       | 0.74          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 2        | 0.74          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 2        | 0.74          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 18       | 0.74          |
| (1,169)  | 2:634:B:LEU:HB2  | 2:700:B:LEU:HD21 | 4        | 0.74          |
| (1,169)  | 2:634:B:LEU:HB2  | 2:700:B:LEU:HD22 | 4        | 0.74          |
| (1,169)  | 2:634:B:LEU:HB2  | 2:700:B:LEU:HD23 | 4        | 0.74          |
| (1,158)  | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG11 | 9        | 0.74          |
| (1,158)  | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG12 | 9        | 0.74          |
| (1,158)  | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG13 | 9        | 0.74          |
| (1,52)   | 2:697:B:LEU:HA   | 2:634:B:LEU:HD11 | 7        | 0.74          |
| (1,52)   | 2:697:B:LEU:HA   | 2:634:B:LEU:HD12 | 7        | 0.74          |
| (1,52)   | 2:697:B:LEU:HA   | 2:634:B:LEU:HD13 | 7        | 0.74          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD2  | 18       | 0.74          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD2  | 18       | 0.74          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD2  | 18       | 0.74          |
| (1,2648) | 1:225:A:LYS:HG3  | 1:224:A:ASN:HA   | 8        | 0.73          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 17       | 0.73          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1739) | 2:691:B:ILE:HG12 | 2:688:B:ASN:HD21 | 7        | 0.73          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 7        | 0.73          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 7        | 0.73          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 7        | 0.73          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 4        | 0.73          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 4        | 0.73          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 4        | 0.73          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD21 | 7        | 0.73          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD22 | 7        | 0.73          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD23 | 7        | 0.73          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 15       | 0.73          |
| (1,537)  | 2:613:B:CYS:HB3  | 2:616:B:GLU:H    | 12       | 0.73          |
| (1,536)  | 2:614:B:GLU:HB2  | 2:615:B:ASP:H    | 3        | 0.73          |
| (1,536)  | 2:634:B:LEU:HG   | 2:634:B:LEU:H    | 6        | 0.73          |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 13       | 0.73          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 8        | 0.73          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 8        | 0.73          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 8        | 0.73          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 14       | 0.73          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 14       | 0.73          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 14       | 0.73          |
| (1,391)  | 2:716:B:LYS:HB2  | 2:716:B:LYS:HE2  | 5        | 0.73          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 19       | 0.73          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 19       | 0.73          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 19       | 0.73          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 3        | 0.73          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 3        | 0.73          |
| (1,197)  | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 6        | 0.73          |
| (1,197)  | 2:641:B:LEU:HD11 | 2:649:B:GLN:HA   | 8        | 0.73          |
| (1,197)  | 2:641:B:LEU:HD12 | 2:649:B:GLN:HA   | 8        | 0.73          |
| (1,197)  | 2:641:B:LEU:HD13 | 2:649:B:GLN:HA   | 8        | 0.73          |
| (1,49)   | 2:649:B:GLN:HA   | 2:641:B:LEU:HD11 | 13       | 0.73          |
| (1,49)   | 2:649:B:GLN:HA   | 2:641:B:LEU:HD12 | 13       | 0.73          |
| (1,49)   | 2:649:B:GLN:HA   | 2:641:B:LEU:HD13 | 13       | 0.73          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 2        | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 2        | 0.72          |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 2        | 0.72          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 5        | 0.72          |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 5        | 0.72          |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 5        | 0.72          |
| (1,2652) | 1:226:A:LEU:HD21 | 1:226:A:LEU:HA   | 10       | 0.72          |
| (1,2652) | 1:226:A:LEU:HD22 | 1:226:A:LEU:HA   | 10       | 0.72          |
| (1,2652) | 1:226:A:LEU:HD23 | 1:226:A:LEU:HA   | 10       | 0.72          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 5        | 0.72          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 6        | 0.72          |
| (1,1682) | 2:606:B:ASN:HB2  | 2:610:B:ILE:HG13 | 11       | 0.72          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 19       | 0.72          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD11 | 16       | 0.72          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD12 | 16       | 0.72          |
| (1,911)  | 2:654:B:LEU:HA   | 2:654:B:LEU:HD13 | 16       | 0.72          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD11 | 8        | 0.72          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD12 | 8        | 0.72          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD13 | 8        | 0.72          |
| (1,750)  | 2:673:B:ILE:HG13 | 2:672:B:ARG:H    | 11       | 0.72          |
| (1,436)  | 1:211:A:LEU:HA   | 2:703:B:LYS:HE2  | 13       | 0.72          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 3        | 0.72          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 3        | 0.72          |
| (1,282)  | 1:207:A:LEU:HD11 | 2:616:B:GLU:HG3  | 4        | 0.72          |
| (1,282)  | 1:207:A:LEU:HD12 | 2:616:B:GLU:HG3  | 4        | 0.72          |
| (1,282)  | 1:207:A:LEU:HD13 | 2:616:B:GLU:HG3  | 4        | 0.72          |
| (1,2197) | 2:677:B:LYS:HE3  | 2:677:B:LYS:H    | 12       | 0.71          |
| (1,761)  | 2:713:B:GLY:HA3  | 1:207:A:LEU:HD21 | 5        | 0.71          |
| (1,761)  | 2:713:B:GLY:HA3  | 1:207:A:LEU:HD22 | 5        | 0.71          |
| (1,761)  | 2:713:B:GLY:HA3  | 1:207:A:LEU:HD23 | 5        | 0.71          |
| (1,698)  | 2:691:B:ILE:HG21 | 2:688:B:ASN:H    | 9        | 0.71          |
| (1,698)  | 2:691:B:ILE:HG22 | 2:688:B:ASN:H    | 9        | 0.71          |
| (1,698)  | 2:691:B:ILE:HG23 | 2:688:B:ASN:H    | 9        | 0.71          |
| (1,456)  | 2:687:B:LYS:HD3  | 2:688:B:ASN:HD21 | 8        | 0.71          |
| (1,456)  | 1:226:A:LEU:HB3  | 2:688:B:ASN:HD21 | 14       | 0.71          |
| (1,432)  | 2:664:B:VAL:HB   | 2:668:B:LYS:HE2  | 19       | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,394)  | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE3  | 3        | 0.71          |
| (1,394)  | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE3  | 3        | 0.71          |
| (1,394)  | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE3  | 3        | 0.71          |
| (1,265)  | 2:697:B:LEU:HD21 | 2:638:B:GLN:HB2  | 13       | 0.71          |
| (1,265)  | 2:697:B:LEU:HD22 | 2:638:B:GLN:HB2  | 13       | 0.71          |
| (1,265)  | 2:697:B:LEU:HD23 | 2:638:B:GLN:HB2  | 13       | 0.71          |
| (1,95)   | 2:662:B:SER:HB3  | 2:665:B:ILE:HD11 | 18       | 0.71          |
| (1,95)   | 2:662:B:SER:HB3  | 2:665:B:ILE:HD12 | 18       | 0.71          |
| (1,95)   | 2:662:B:SER:HB3  | 2:665:B:ILE:HD13 | 18       | 0.71          |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD21 | 15       | 0.7           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD22 | 15       | 0.7           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD23 | 15       | 0.7           |
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 3        | 0.7           |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 3        | 0.7           |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 3        | 0.7           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 13       | 0.7           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 13       | 0.7           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 13       | 0.7           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 20       | 0.7           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 20       | 0.7           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 20       | 0.7           |
| (1,829)  | 2:677:B:LYS:HD3  | 2:677:B:LYS:HA   | 15       | 0.7           |
| (1,432)  | 2:720:B:GLU:HB3  | 2:724:B:LYS:HE2  | 3        | 0.7           |
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD2  | 4        | 0.7           |
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD2  | 7        | 0.7           |
| (1,389)  | 2:677:B:LYS:HG2  | 2:677:B:LYS:HE2  | 3        | 0.7           |
| (1,267)  | 2:637:B:ILE:HD11 | 2:640:B:LYS:HD3  | 3        | 0.7           |
| (1,267)  | 2:637:B:ILE:HD12 | 2:640:B:LYS:HD3  | 3        | 0.7           |
| (1,267)  | 2:637:B:ILE:HD13 | 2:640:B:LYS:HD3  | 3        | 0.7           |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 1        | 0.7           |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD11 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD12 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD13 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD11 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD12 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD13 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD11 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD12 | 9        | 0.69          |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD13 | 9        | 0.69          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 18       | 0.69          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 18       | 0.69          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 18       | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1992) | 2:633:B:VAL:HG11 | 2:633:B:VAL:H    | 7        | 0.69          |
| (1,1992) | 2:633:B:VAL:HG12 | 2:633:B:VAL:H    | 7        | 0.69          |
| (1,1992) | 2:633:B:VAL:HG13 | 2:633:B:VAL:H    | 7        | 0.69          |
| (1,1908) | 2:617:B:ARG:HG3  | 2:616:B:GLU:H    | 10       | 0.69          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD11 | 4        | 0.69          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD12 | 4        | 0.69          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD13 | 4        | 0.69          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD11 | 13       | 0.69          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD12 | 13       | 0.69          |
| (1,890)  | 2:700:B:LEU:HA   | 2:700:B:LEU:HD13 | 13       | 0.69          |
| (1,619)  | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 12       | 0.69          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 4        | 0.69          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 4        | 0.69          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 1        | 0.69          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 1        | 0.69          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 1        | 0.69          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 15       | 0.69          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD3  | 9        | 0.69          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD3  | 9        | 0.69          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD3  | 9        | 0.69          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 6        | 0.68          |
| (1,1992) | 2:633:B:VAL:HG11 | 2:633:B:VAL:H    | 4        | 0.68          |
| (1,1992) | 2:633:B:VAL:HG12 | 2:633:B:VAL:H    | 4        | 0.68          |
| (1,1992) | 2:633:B:VAL:HG13 | 2:633:B:VAL:H    | 4        | 0.68          |
| (1,1682) | 2:606:B:ASN:HB2  | 2:610:B:ILE:HG13 | 18       | 0.68          |
| (1,1599) | 2:668:B:LYS:HG2  | 2:668:B:LYS:HE2  | 5        | 0.68          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 18       | 0.68          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 18       | 0.68          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 18       | 0.68          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 18       | 0.68          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 18       | 0.68          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 18       | 0.68          |
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD3  | 10       | 0.68          |
| (1,394)  | 2:717:B:VAL:HG21 | 2:716:B:LYS:HE3  | 17       | 0.68          |
| (1,394)  | 2:717:B:VAL:HG22 | 2:716:B:LYS:HE3  | 17       | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,394)  | 2:717:B:VAL:HG23 | 2:716:B:LYS:HE3  | 17       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD21 | 2:630:B:THR:HG21 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD21 | 2:630:B:THR:HG22 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD21 | 2:630:B:THR:HG23 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD22 | 2:630:B:THR:HG21 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD22 | 2:630:B:THR:HG22 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD22 | 2:630:B:THR:HG23 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD23 | 2:630:B:THR:HG21 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD23 | 2:630:B:THR:HG22 | 11       | 0.68          |
| (1,256)  | 2:658:B:LEU:HD23 | 2:630:B:THR:HG23 | 11       | 0.68          |
| (1,214)  | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 13       | 0.68          |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG11 | 7        | 0.68          |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG12 | 7        | 0.68          |
| (1,131)  | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG13 | 7        | 0.68          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD21 | 14       | 0.67          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD22 | 14       | 0.67          |
| (1,2507) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD23 | 14       | 0.67          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 11       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 10       | 0.67          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 10       | 0.67          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD21 | 11       | 0.67          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD22 | 11       | 0.67          |
| (1,1166) | 2:711:B:GLN:HG2  | 2:624:B:LEU:HD23 | 11       | 0.67          |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD11 | 11       | 0.67          |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD12 | 11       | 0.67          |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD13 | 11       | 0.67          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 13       | 0.67          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 13       | 0.67          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 13       | 0.67          |
| (1,711)  | 2:670:B:LEU:HD21 | 2:675:B:ALA:H    | 14       | 0.67          |
| (1,711)  | 2:670:B:LEU:HD22 | 2:675:B:ALA:H    | 14       | 0.67          |
| (1,711)  | 2:670:B:LEU:HD23 | 2:675:B:ALA:H    | 14       | 0.67          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 11       | 0.67          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 11       | 0.67          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 11       | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB1  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB2  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB3  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB1  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB2  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB3  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB1  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB2  | 14       | 0.67          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB3  | 14       | 0.67          |
| (1,251)  | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB1  | 1        | 0.67          |
| (1,251)  | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB2  | 1        | 0.67          |
| (1,251)  | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB3  | 1        | 0.67          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE1  | 18       | 0.67          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE2  | 18       | 0.67          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE3  | 18       | 0.67          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 8        | 0.67          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 13       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD11 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD12 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD13 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD11 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD12 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD13 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD11 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD12 | 14       | 0.67          |
| (1,192)  | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD13 | 14       | 0.67          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD11 | 4        | 0.67          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD12 | 4        | 0.67          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD13 | 4        | 0.67          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD21 | 20       | 0.66          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD22 | 20       | 0.66          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD23 | 20       | 0.66          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD21 | 20       | 0.66          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD22 | 20       | 0.66          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD23 | 20       | 0.66          |
| (1,1713) | 2:686:B:ARG:HD3  | 2:683:B:ASP:HA   | 1        | 0.66          |
| (1,756)  | 2:620:B:LEU:HD21 | 2:707:B:TRP:HE1  | 5        | 0.66          |
| (1,756)  | 2:620:B:LEU:HD22 | 2:707:B:TRP:HE1  | 5        | 0.66          |
| (1,756)  | 2:620:B:LEU:HD23 | 2:707:B:TRP:HE1  | 5        | 0.66          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 5        | 0.66          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 5        | 0.66          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 5        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 6        | 0.66          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 5        | 0.66          |
| (1,660)  | 2:671:B:GLN:HB2  | 2:675:B:ALA:H    | 17       | 0.66          |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 9        | 0.66          |
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD3  | 9        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE1  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE2  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE3  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE1  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE2  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE3  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE1  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE2  | 6        | 0.66          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE3  | 6        | 0.66          |
| (1,394)  | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE3  | 4        | 0.66          |
| (1,394)  | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE3  | 4        | 0.66          |
| (1,394)  | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE3  | 4        | 0.66          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 18       | 0.66          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 18       | 0.66          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 18       | 0.66          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 15       | 0.66          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 15       | 0.66          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 15       | 0.66          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 9        | 0.66          |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD21 | 3        | 0.66          |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD22 | 3        | 0.66          |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD23 | 3        | 0.66          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 6        | 0.65          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 6        | 0.65          |
| (1,1642) | 1:211:A:LEU:HD21 | 2:702:B:MET:HE1  | 13       | 0.65          |
| (1,1642) | 1:211:A:LEU:HD21 | 2:702:B:MET:HE2  | 13       | 0.65          |
| (1,1642) | 1:211:A:LEU:HD21 | 2:702:B:MET:HE3  | 13       | 0.65          |
| (1,1642) | 1:211:A:LEU:HD22 | 2:702:B:MET:HE1  | 13       | 0.65          |
| (1,1642) | 1:211:A:LEU:HD22 | 2:702:B:MET:HE2  | 13       | 0.65          |
| (1,1642) | 1:211:A:LEU:HD22 | 2:702:B:MET:HE3  | 13       | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1642) | 1:211:A:LEU:HD23 | 2:702:B:MET:HE1  | 13       | 0.65          |
| (1,1642) | 1:211:A:LEU:HD23 | 2:702:B:MET:HE2  | 13       | 0.65          |
| (1,1642) | 1:211:A:LEU:HD23 | 2:702:B:MET:HE3  | 13       | 0.65          |
| (1,1559) | 2:716:B:LYS:HG2  | 2:716:B:LYS:HA   | 8        | 0.65          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 6        | 0.65          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 6        | 0.65          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 6        | 0.65          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD21 | 7        | 0.65          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD22 | 7        | 0.65          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD23 | 7        | 0.65          |
| (1,899)  | 2:620:B:LEU:HA   | 2:623:B:VAL:HG11 | 5        | 0.65          |
| (1,899)  | 2:620:B:LEU:HA   | 2:623:B:VAL:HG12 | 5        | 0.65          |
| (1,899)  | 2:620:B:LEU:HA   | 2:623:B:VAL:HG13 | 5        | 0.65          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 17       | 0.65          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 17       | 0.65          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 17       | 0.65          |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 5        | 0.65          |
| (1,660)  | 2:672:B:ARG:HB3  | 2:675:B:ALA:H    | 2        | 0.65          |
| (1,535)  | 2:716:B:LYS:HD2  | 2:720:B:GLU:H    | 17       | 0.65          |
| (1,456)  | 1:226:A:LEU:HB3  | 2:688:B:ASN:HD21 | 10       | 0.65          |
| (1,391)  | 2:716:B:LYS:HB3  | 2:716:B:LYS:HE2  | 6        | 0.65          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB2  | 2        | 0.65          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB2  | 2        | 0.65          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB2  | 2        | 0.65          |
| (1,267)  | 2:637:B:ILE:HD11 | 2:640:B:LYS:HD2  | 11       | 0.65          |
| (1,267)  | 2:637:B:ILE:HD12 | 2:640:B:LYS:HD2  | 11       | 0.65          |
| (1,267)  | 2:637:B:ILE:HD13 | 2:640:B:LYS:HD2  | 11       | 0.65          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 7        | 0.65          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 7        | 0.65          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 7        | 0.65          |
| (1,179)  | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG21 | 12       | 0.65          |
| (1,179)  | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG22 | 12       | 0.65          |
| (1,179)  | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG23 | 12       | 0.65          |
| (1,131)  | 2:672:B:ARG:HD2  | 2:623:B:VAL:HG11 | 17       | 0.65          |
| (1,131)  | 2:672:B:ARG:HD2  | 2:623:B:VAL:HG12 | 17       | 0.65          |
| (1,131)  | 2:672:B:ARG:HD2  | 2:623:B:VAL:HG13 | 17       | 0.65          |
| (1,51)   | 2:652:B:PHE:HB2  | 2:644:B:LEU:HD21 | 19       | 0.65          |
| (1,51)   | 2:652:B:PHE:HB2  | 2:644:B:LEU:HD22 | 19       | 0.65          |
| (1,51)   | 2:652:B:PHE:HB2  | 2:644:B:LEU:HD23 | 19       | 0.65          |
| (1,1892) | 2:612:B:ARG:HG2  | 2:612:B:ARG:H    | 19       | 0.64          |
| (1,1631) | 1:211:A:LEU:HD11 | 2:703:B:LYS:HE2  | 20       | 0.64          |
| (1,1631) | 1:211:A:LEU:HD12 | 2:703:B:LYS:HE2  | 20       | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1631) | 1:211:A:LEU:HD13 | 2:703:B:LYS:HE2  | 20       | 0.64          |
| (1,1423) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HG3  | 16       | 0.64          |
| (1,1423) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HG3  | 16       | 0.64          |
| (1,1423) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HG3  | 16       | 0.64          |
| (1,535)  | 2:719:B:ARG:HG3  | 2:720:B:GLU:H    | 9        | 0.64          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 18       | 0.64          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 18       | 0.64          |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 18       | 0.64          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB2  | 10       | 0.64          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB2  | 10       | 0.64          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB2  | 10       | 0.64          |
| (1,279)  | 2:620:B:LEU:HD11 | 2:711:B:GLN:HG2  | 17       | 0.64          |
| (1,279)  | 2:620:B:LEU:HD12 | 2:711:B:GLN:HG2  | 17       | 0.64          |
| (1,279)  | 2:620:B:LEU:HD13 | 2:711:B:GLN:HG2  | 17       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 19       | 0.64          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 19       | 0.64          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE1  | 2        | 0.64          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE2  | 2        | 0.64          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE3  | 2        | 0.64          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 2        | 0.64          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 14       | 0.63          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 14       | 0.63          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 17       | 0.63          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 17       | 0.63          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 17       | 0.63          |
| (1,672)  | 2:675:B:ALA:HB1  | 2:678:B:ALA:H    | 16       | 0.63          |
| (1,672)  | 2:675:B:ALA:HB2  | 2:678:B:ALA:H    | 16       | 0.63          |
| (1,672)  | 2:675:B:ALA:HB3  | 2:678:B:ALA:H    | 16       | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD3  | 5        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD11 | 2:673:B:ILE:HG21 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD11 | 2:673:B:ILE:HG22 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD11 | 2:673:B:ILE:HG23 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD12 | 2:673:B:ILE:HG21 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD12 | 2:673:B:ILE:HG22 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD12 | 2:673:B:ILE:HG23 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD13 | 2:673:B:ILE:HG21 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD13 | 2:673:B:ILE:HG22 | 4        | 0.63          |
| (1,418)  | 1:210:A:LEU:HD13 | 2:673:B:ILE:HG23 | 4        | 0.63          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE1  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE2  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE3  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE1  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE2  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE3  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE1  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE2  | 18       | 0.63          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE3  | 18       | 0.63          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE1  | 3        | 0.63          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE2  | 3        | 0.63          |
| (1,249)  | 1:211:A:LEU:HB3  | 2:702:B:MET:HE3  | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG11 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG12 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG13 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG11 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG12 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG13 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG11 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG12 | 3        | 0.63          |
| (1,187)  | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG13 | 3        | 0.63          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG11 | 12       | 0.62          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG12 | 12       | 0.62          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG13 | 12       | 0.62          |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 5        | 0.62          |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG21 | 16       | 0.62          |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG22 | 16       | 0.62          |
| (2,3)    | 2:707:B:TRP:HZ3  | 2:623:B:VAL:HG23 | 16       | 0.62          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD21 | 20       | 0.62          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD22 | 20       | 0.62          |
| (1,2505) | 2:673:B:ILE:HA   | 1:210:A:LEU:HD23 | 20       | 0.62          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 18       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 6        | 0.62          |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG11 | 4        | 0.62          |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG12 | 4        | 0.62          |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG13 | 4        | 0.62          |
| (1,574)  | 2:631:B:ILE:HG21 | 2:630:B:THR:H    | 16       | 0.62          |
| (1,574)  | 2:631:B:ILE:HG22 | 2:630:B:THR:H    | 16       | 0.62          |
| (1,574)  | 2:631:B:ILE:HG23 | 2:630:B:THR:H    | 16       | 0.62          |
| (1,319)  | 2:687:B:LYS:HA   | 2:653:B:ARG:HD2  | 3        | 0.62          |
| (1,298)  | 1:207:A:LEU:HG   | 2:710:B:ALA:HB1  | 15       | 0.62          |
| (1,298)  | 1:207:A:LEU:HG   | 2:710:B:ALA:HB2  | 15       | 0.62          |
| (1,298)  | 1:207:A:LEU:HG   | 2:710:B:ALA:HB3  | 15       | 0.62          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 11       | 0.62          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 11       | 0.62          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 11       | 0.62          |
| (1,206)  | 2:686:B:ARG:HG2  | 2:653:B:ARG:HG2  | 5        | 0.62          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD11 | 8        | 0.62          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD12 | 8        | 0.62          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD13 | 8        | 0.62          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD11 | 8        | 0.62          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD12 | 8        | 0.62          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD13 | 8        | 0.62          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 4        | 0.61          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 4        | 0.61          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 6        | 0.61          |
| (1,599)  | 2:634:B:LEU:HD21 | 2:637:B:ILE:H    | 4        | 0.61          |
| (1,599)  | 2:634:B:LEU:HD22 | 2:637:B:ILE:H    | 4        | 0.61          |
| (1,599)  | 2:634:B:LEU:HD23 | 2:637:B:ILE:H    | 4        | 0.61          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 19       | 0.61          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 19       | 0.61          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 19       | 0.61          |
| (1,432)  | 2:700:B:LEU:HG   | 2:701:B:LYS:HE3  | 12       | 0.61          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB1  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB2  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB3  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB1  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB2  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB3  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB1  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB2  | 6        | 0.61          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB3  | 6        | 0.61          |
| (1,260)  | 2:717:B:VAL:HG11 | 2:719:B:ARG:HG3  | 16       | 0.61          |
| (1,260)  | 2:717:B:VAL:HG12 | 2:719:B:ARG:HG3  | 16       | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,260)  | 2:717:B:VAL:HG13 | 2:719:B:ARG:HG3  | 16       | 0.61          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE1  | 15       | 0.61          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE2  | 15       | 0.61          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE3  | 15       | 0.61          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 19       | 0.61          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 19       | 0.61          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 19       | 0.61          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 15       | 0.61          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 15       | 0.61          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 15       | 0.61          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD21 | 16       | 0.6           |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD22 | 16       | 0.6           |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD23 | 16       | 0.6           |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 5        | 0.6           |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 18       | 0.6           |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 18       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 14       | 0.6           |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 14       | 0.6           |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 17       | 0.6           |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 17       | 0.6           |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 17       | 0.6           |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 3        | 0.6           |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 1        | 0.6           |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 7        | 0.6           |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 7        | 0.6           |
| (1,441)  | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 7        | 0.6           |
| (1,436)  | 1:211:A:LEU:HA   | 2:703:B:LYS:HE2  | 20       | 0.6           |
| (1,432)  | 2:700:B:LEU:HG   | 2:701:B:LYS:HE2  | 9        | 0.6           |
| (1,429)  | 2:698:B:LYS:HA   | 2:698:B:LYS:HD2  | 18       | 0.6           |
| (1,396)  | 2:632:B:ARG:HB2  | 2:632:B:ARG:HD2  | 5        | 0.6           |
| (1,238)  | 2:646:B:ALA:HB1  | 2:647:B:GLU:HG2  | 2        | 0.6           |
| (1,238)  | 2:646:B:ALA:HB2  | 2:647:B:GLU:HG2  | 2        | 0.6           |
| (1,238)  | 2:646:B:ALA:HB3  | 2:647:B:GLU:HG2  | 2        | 0.6           |
| (1,16)   | 2:624:B:LEU:HD21 | 2:708:B:ARG:HD2  | 5        | 0.6           |
| (1,16)   | 2:624:B:LEU:HD22 | 2:708:B:ARG:HD2  | 5        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,16)   | 2:624:B:LEU:HD23 | 2:708:B:ARG:HD2  | 5        | 0.6           |
| (1,15)   | 2:664:B:VAL:HG21 | 2:667:B:ARG:HD3  | 18       | 0.6           |
| (1,15)   | 2:664:B:VAL:HG22 | 2:667:B:ARG:HD3  | 18       | 0.6           |
| (1,15)   | 2:664:B:VAL:HG23 | 2:667:B:ARG:HD3  | 18       | 0.6           |
| (1,14)   | 2:658:B:LEU:HD11 | 2:686:B:ARG:HD2  | 10       | 0.6           |
| (1,14)   | 2:658:B:LEU:HD12 | 2:686:B:ARG:HD2  | 10       | 0.6           |
| (1,14)   | 2:658:B:LEU:HD13 | 2:686:B:ARG:HD2  | 10       | 0.6           |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD11 | 3        | 0.59          |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD12 | 3        | 0.59          |
| (2,6)    | 2:658:B:LEU:HG   | 2:634:B:LEU:HD13 | 3        | 0.59          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 13       | 0.59          |
| (1,1351) | 2:716:B:LYS:HE2  | 2:720:B:GLU:HG3  | 8        | 0.59          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 17       | 0.59          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 18       | 0.59          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 7        | 0.59          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 7        | 0.59          |
| (1,698)  | 2:691:B:ILE:HG21 | 2:688:B:ASN:H    | 3        | 0.59          |
| (1,698)  | 2:691:B:ILE:HG22 | 2:688:B:ASN:H    | 3        | 0.59          |
| (1,698)  | 2:691:B:ILE:HG23 | 2:688:B:ASN:H    | 3        | 0.59          |
| (1,656)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:H    | 3        | 0.59          |
| (1,656)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:H    | 3        | 0.59          |
| (1,656)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:H    | 3        | 0.59          |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 5        | 0.59          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 15       | 0.59          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 15       | 0.59          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 15       | 0.59          |
| (1,444)  | 2:670:B:LEU:HG   | 2:658:B:LEU:HD21 | 8        | 0.59          |
| (1,444)  | 2:670:B:LEU:HG   | 2:658:B:LEU:HD22 | 8        | 0.59          |
| (1,444)  | 2:670:B:LEU:HG   | 2:658:B:LEU:HD23 | 8        | 0.59          |
| (1,359)  | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 5        | 0.59          |
| (1,214)  | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 9        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD11 | 4        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD12 | 4        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD13 | 4        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD11 | 4        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,192)  | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD12 | 4        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD13 | 4        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD11 | 4        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD12 | 4        | 0.59          |
| (1,192)  | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD13 | 4        | 0.59          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 17       | 0.59          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 17       | 0.59          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 17       | 0.59          |
| (1,174)  | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD11 | 18       | 0.59          |
| (1,174)  | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD12 | 18       | 0.59          |
| (1,174)  | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD13 | 18       | 0.59          |
| (1,2125) | 2:613:B:CYS:HB3  | 2:615:B:ASP:H    | 20       | 0.58          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 3        | 0.58          |
| (1,1908) | 2:617:B:ARG:HG2  | 2:616:B:GLU:H    | 17       | 0.58          |
| (1,1442) | 2:652:B:PHE:HE1  | 2:640:B:LYS:HD3  | 3        | 0.58          |
| (1,1442) | 2:652:B:PHE:HE2  | 2:640:B:LYS:HD3  | 3        | 0.58          |
| (1,1354) | 2:716:B:LYS:HD2  | 2:720:B:GLU:HG3  | 16       | 0.58          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 16       | 0.58          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 16       | 0.58          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 16       | 0.58          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 15       | 0.58          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 15       | 0.58          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 15       | 0.58          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB1  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB2  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB3  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB1  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB2  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB3  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB1  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB2  | 4        | 0.58          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB3  | 4        | 0.58          |
| (1,271)  | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD3  | 2        | 0.58          |
| (1,271)  | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD3  | 2        | 0.58          |
| (1,271)  | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD3  | 2        | 0.58          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 3        | 0.58          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 3        | 0.58          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 3        | 0.58          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG21 | 9        | 0.58          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG22 | 9        | 0.58          |
| (1,179)  | 2:628:B:LEU:HG   | 2:631:B:ILE:HG23 | 9        | 0.58          |
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD11 | 3        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD12 | 3        | 0.58          |
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD13 | 3        | 0.58          |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD11 | 3        | 0.58          |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD12 | 3        | 0.58          |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD13 | 3        | 0.58          |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD11 | 3        | 0.58          |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD12 | 3        | 0.58          |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD13 | 3        | 0.58          |
| (1,15)   | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD2  | 11       | 0.58          |
| (1,15)   | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD2  | 11       | 0.58          |
| (1,15)   | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD2  | 11       | 0.58          |
| (1,12)   | 2:611:B:TYR:HD1  | 2:616:B:GLU:HA   | 9        | 0.58          |
| (1,12)   | 2:611:B:TYR:HD2  | 2:616:B:GLU:HA   | 9        | 0.58          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD21 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD22 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD23 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD21 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD22 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD23 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD21 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD22 | 4        | 0.57          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD23 | 4        | 0.57          |
| (1,1704) | 2:711:B:GLN:HG2  | 2:711:B:GLN:HA   | 10       | 0.57          |
| (1,1631) | 1:211:A:LEU:HD11 | 2:703:B:LYS:HE2  | 9        | 0.57          |
| (1,1631) | 1:211:A:LEU:HD12 | 2:703:B:LYS:HE2  | 9        | 0.57          |
| (1,1631) | 1:211:A:LEU:HD13 | 2:703:B:LYS:HE2  | 9        | 0.57          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 8        | 0.57          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 8        | 0.57          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 8        | 0.57          |
| (1,574)  | 2:631:B:ILE:HG21 | 2:630:B:THR:H    | 12       | 0.57          |
| (1,574)  | 2:631:B:ILE:HG22 | 2:630:B:THR:H    | 12       | 0.57          |
| (1,574)  | 2:631:B:ILE:HG23 | 2:630:B:THR:H    | 12       | 0.57          |
| (1,574)  | 2:631:B:ILE:HG21 | 2:630:B:THR:H    | 18       | 0.57          |
| (1,574)  | 2:631:B:ILE:HG22 | 2:630:B:THR:H    | 18       | 0.57          |
| (1,574)  | 2:631:B:ILE:HG23 | 2:630:B:THR:H    | 18       | 0.57          |
| (1,429)  | 2:717:B:VAL:HA   | 2:716:B:LYS:HD2  | 11       | 0.57          |
| (1,237)  | 2:613:B:CYS:HB3  | 2:614:B:GLU:HG3  | 12       | 0.57          |
| (1,197)  | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 1        | 0.57          |
| (1,2310) | 2:616:B:GLU:HB3  | 2:616:B:GLU:H    | 9        | 0.56          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 17       | 0.56          |
| (1,1852) | 2:701:B:LYS:HD2  | 2:700:B:LEU:H    | 8        | 0.56          |
| (1,1626) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HA   | 4        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1626) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HA   | 4        | 0.56          |
| (1,1626) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HA   | 4        | 0.56          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 17       | 0.56          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 17       | 0.56          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 17       | 0.56          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 6        | 0.56          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 6        | 0.56          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 6        | 0.56          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 11       | 0.56          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 11       | 0.56          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 11       | 0.56          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 18       | 0.56          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 18       | 0.56          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 18       | 0.56          |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 7        | 0.56          |
| (1,574)  | 2:631:B:ILE:HG21 | 2:630:B:THR:H    | 3        | 0.56          |
| (1,574)  | 2:631:B:ILE:HG22 | 2:630:B:THR:H    | 3        | 0.56          |
| (1,574)  | 2:631:B:ILE:HG23 | 2:630:B:THR:H    | 3        | 0.56          |
| (1,535)  | 2:654:B:LEU:HB2  | 2:655:B:ASP:H    | 20       | 0.56          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 20       | 0.56          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 20       | 0.56          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 20       | 0.56          |
| (1,466)  | 2:654:B:LEU:HA   | 2:659:B:GLY:H    | 1        | 0.56          |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 8        | 0.56          |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG21 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG22 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG23 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG21 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG22 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG23 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG21 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG22 | 13       | 0.56          |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG23 | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB1  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB2  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB3  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB1  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB2  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB3  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB1  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB2  | 13       | 0.56          |
| (1,299)  | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB3  | 13       | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD21 | 8        | 0.56          |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD22 | 8        | 0.56          |
| (1,170)  | 2:631:B:ILE:HG13 | 2:700:B:LEU:HD23 | 8        | 0.56          |
| (1,19)   | 2:682:B:ILE:HG21 | 2:681:B:ILE:HA   | 5        | 0.56          |
| (1,19)   | 2:682:B:ILE:HG22 | 2:681:B:ILE:HA   | 5        | 0.56          |
| (1,19)   | 2:682:B:ILE:HG23 | 2:681:B:ILE:HA   | 5        | 0.56          |
| (1,12)   | 2:611:B:TYR:HD1  | 2:614:B:GLU:HA   | 1        | 0.56          |
| (1,12)   | 2:611:B:TYR:HD2  | 2:614:B:GLU:HA   | 1        | 0.56          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 17       | 0.55          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 17       | 0.55          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 17       | 0.55          |
| (1,1740) | 2:691:B:ILE:HG12 | 2:688:B:ASN:HD22 | 17       | 0.55          |
| (1,1489) | 2:653:B:ARG:HD2  | 2:687:B:LYS:HA   | 16       | 0.55          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD11 | 16       | 0.55          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD12 | 16       | 0.55          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD13 | 16       | 0.55          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 16       | 0.55          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 16       | 0.55          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 16       | 0.55          |
| (1,1004) | 2:712:B:ARG:HD2  | 2:712:B:ARG:HB2  | 1        | 0.55          |
| (1,937)  | 2:669:B:ALA:HA   | 2:668:B:LYS:HG3  | 13       | 0.55          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD21 | 13       | 0.55          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD22 | 13       | 0.55          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD23 | 13       | 0.55          |
| (1,684)  | 2:716:B:LYS:HD3  | 2:717:B:VAL:H    | 15       | 0.55          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 2        | 0.55          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 2        | 0.55          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 2        | 0.55          |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 17       | 0.55          |
| (1,401)  | 2:719:B:ARG:HB2  | 2:719:B:ARG:HD3  | 8        | 0.55          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 17       | 0.55          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 17       | 0.55          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 17       | 0.55          |
| (1,274)  | 2:695:B:ILE:HD11 | 2:694:B:PRO:HB2  | 5        | 0.55          |
| (1,274)  | 2:695:B:ILE:HD12 | 2:694:B:PRO:HB2  | 5        | 0.55          |
| (1,274)  | 2:695:B:ILE:HD13 | 2:694:B:PRO:HB2  | 5        | 0.55          |
| (1,260)  | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 4        | 0.55          |
| (1,260)  | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 4        | 0.55          |
| (1,260)  | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 4        | 0.55          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 19       | 0.55          |
| (1,182)  | 2:678:B:ALA:HB1  | 2:682:B:ILE:HG21 | 9        | 0.55          |
| (1,182)  | 2:678:B:ALA:HB1  | 2:682:B:ILE:HG22 | 9        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,182)  | 2:678:B:ALA:HB1  | 2:682:B:ILE:HG23 | 9        | 0.55          |
| (1,182)  | 2:678:B:ALA:HB2  | 2:682:B:ILE:HG21 | 9        | 0.55          |
| (1,182)  | 2:678:B:ALA:HB2  | 2:682:B:ILE:HG22 | 9        | 0.55          |
| (1,182)  | 2:678:B:ALA:HB2  | 2:682:B:ILE:HG23 | 9        | 0.55          |
| (1,182)  | 2:678:B:ALA:HB3  | 2:682:B:ILE:HG21 | 9        | 0.55          |
| (1,182)  | 2:678:B:ALA:HB3  | 2:682:B:ILE:HG22 | 9        | 0.55          |
| (1,182)  | 2:678:B:ALA:HB3  | 2:682:B:ILE:HG23 | 9        | 0.55          |
| (1,151)  | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD11 | 5        | 0.55          |
| (1,151)  | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD12 | 5        | 0.55          |
| (1,151)  | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD13 | 5        | 0.55          |
| (1,151)  | 2:641:B:LEU:HG   | 2:654:B:LEU:HD11 | 11       | 0.55          |
| (1,151)  | 2:641:B:LEU:HG   | 2:654:B:LEU:HD12 | 11       | 0.55          |
| (1,151)  | 2:641:B:LEU:HG   | 2:654:B:LEU:HD13 | 11       | 0.55          |
| (1,19)   | 2:682:B:ILE:HG21 | 2:681:B:ILE:HA   | 7        | 0.55          |
| (1,19)   | 2:682:B:ILE:HG22 | 2:681:B:ILE:HA   | 7        | 0.55          |
| (1,19)   | 2:682:B:ILE:HG23 | 2:681:B:ILE:HA   | 7        | 0.55          |
| (1,16)   | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD2  | 20       | 0.55          |
| (1,16)   | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD2  | 20       | 0.55          |
| (1,16)   | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD2  | 20       | 0.55          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD21 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD22 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD23 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD21 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD22 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD23 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD21 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD22 | 17       | 0.54          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD23 | 17       | 0.54          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 2        | 0.54          |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 3        | 0.54          |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 19       | 0.54          |
| (1,977)  | 2:642:B:SER:HB3  | 2:643:B:ARG:HG3  | 2        | 0.54          |
| (1,937)  | 2:669:B:ALA:HA   | 2:668:B:LYS:HG3  | 5        | 0.54          |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD11 | 4        | 0.54          |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD12 | 4        | 0.54          |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD13 | 4        | 0.54          |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD11 | 11       | 0.54          |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD12 | 11       | 0.54          |
| (1,912)  | 2:670:B:LEU:HA   | 2:670:B:LEU:HD13 | 11       | 0.54          |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG11 | 7        | 0.54          |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG12 | 7        | 0.54          |
| (1,905)  | 2:630:B:THR:HA   | 2:633:B:VAL:HG13 | 7        | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 18       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 8        | 0.54          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 17       | 0.54          |
| (1,256)  | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 17       | 0.54          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 17       | 0.54          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 15       | 0.54          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 15       | 0.54          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 15       | 0.54          |
| (1,155)  | 2:638:B:GLN:HG3  | 2:641:B:LEU:HD11 | 4        | 0.54          |
| (1,155)  | 2:638:B:GLN:HG3  | 2:641:B:LEU:HD12 | 4        | 0.54          |
| (1,155)  | 2:638:B:GLN:HG3  | 2:641:B:LEU:HD13 | 4        | 0.54          |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD3  | 11       | 0.54          |
| (1,63)   | 2:630:B:THR:HA   | 2:632:B:ARG:HG3  | 7        | 0.54          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 2        | 0.54          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 2        | 0.54          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 2        | 0.54          |
| (1,2239) | 2:687:B:LYS:HE2  | 2:684:B:GLY:H    | 5        | 0.53          |
| (1,1599) | 2:668:B:LYS:HG2  | 2:668:B:LYS:HE2  | 13       | 0.53          |
| (1,1026) | 2:706:B:GLU:HA   | 2:709:B:GLU:HG3  | 5        | 0.53          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD11 | 3        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD12 | 3        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD13 | 3        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD11 | 6        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD12 | 6        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD13 | 6        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD11 | 8        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD12 | 8        | 0.53          |
| (1,912) | 2:670:B:LEU:HA   | 2:670:B:LEU:HD13 | 8        | 0.53          |
| (1,698) | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 20       | 0.53          |
| (1,698) | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 20       | 0.53          |
| (1,698) | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 20       | 0.53          |
| (1,672) | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 17       | 0.53          |
| (1,535) | 2:719:B:ARG:HG3  | 2:720:B:GLU:H    | 16       | 0.53          |
| (1,392) | 2:631:B:ILE:HG21 | 2:701:B:LYS:HE3  | 20       | 0.53          |
| (1,392) | 2:631:B:ILE:HG22 | 2:701:B:LYS:HE3  | 20       | 0.53          |
| (1,392) | 2:631:B:ILE:HG23 | 2:701:B:LYS:HE3  | 20       | 0.53          |
| (1,389) | 2:687:B:LYS:HG3  | 2:687:B:LYS:HE3  | 5        | 0.53          |
| (1,278) | 2:685:B:LEU:HD11 | 2:696:B:VAL:HB   | 5        | 0.53          |
| (1,278) | 2:685:B:LEU:HD12 | 2:696:B:VAL:HB   | 5        | 0.53          |
| (1,278) | 2:685:B:LEU:HD13 | 2:696:B:VAL:HB   | 5        | 0.53          |
| (1,266) | 2:658:B:LEU:HD11 | 2:634:B:LEU:HG   | 18       | 0.53          |
| (1,266) | 2:658:B:LEU:HD12 | 2:634:B:LEU:HG   | 18       | 0.53          |
| (1,266) | 2:658:B:LEU:HD13 | 2:634:B:LEU:HG   | 18       | 0.53          |
| (1,260) | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 14       | 0.53          |
| (1,260) | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 14       | 0.53          |
| (1,260) | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 14       | 0.53          |
| (1,256) | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 13       | 0.53          |
| (1,256) | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 13       | 0.53          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 13       | 0.53          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 13       | 0.53          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 13       | 0.53          |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 12       | 0.53          |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 12       | 0.53          |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 12       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG21 | 13       | 0.53          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG22 | 13       | 0.53          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG23 | 13       | 0.53          |
| (1,66)   | 2:636:B:ALA:HA   | 2:639:B:LYS:HD3  | 19       | 0.53          |
| (1,19)   | 2:682:B:ILE:HG21 | 2:681:B:ILE:HA   | 12       | 0.53          |
| (1,19)   | 2:682:B:ILE:HG22 | 2:681:B:ILE:HA   | 12       | 0.53          |
| (1,19)   | 2:682:B:ILE:HG23 | 2:681:B:ILE:HA   | 12       | 0.53          |
| (2,14)   | 1:220:A:LEU:HD21 | 1:217:A:MET:HG2  | 16       | 0.52          |
| (2,14)   | 1:220:A:LEU:HD22 | 1:217:A:MET:HG2  | 16       | 0.52          |
| (2,14)   | 1:220:A:LEU:HD23 | 1:217:A:MET:HG2  | 16       | 0.52          |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 9        | 0.52          |
| (1,2310) | 2:616:B:GLU:HB3  | 2:616:B:GLU:H    | 17       | 0.52          |
| (1,2058) | 2:645:B:SER:HB2  | 2:645:B:SER:H    | 18       | 0.52          |
| (1,1852) | 2:701:B:LYS:HD2  | 2:700:B:LEU:H    | 20       | 0.52          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB1  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB2  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB3  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB1  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB2  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB3  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB1  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB2  | 3        | 0.52          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB3  | 3        | 0.52          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD11 | 5        | 0.52          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD12 | 5        | 0.52          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD13 | 5        | 0.52          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 1        | 0.52          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 1        | 0.52          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 1        | 0.52          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 15       | 0.52          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 15       | 0.52          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 15       | 0.52          |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 1        | 0.52          |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 18       | 0.52          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 9        | 0.52          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 9        | 0.52          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 9        | 0.52          |
| (1,429)  | 2:717:B:VAL:HA   | 2:716:B:LYS:HD2  | 6        | 0.52          |
| (1,420)  | 2:682:B:ILE:HG13 | 2:681:B:ILE:HD11 | 6        | 0.52          |
| (1,420)  | 2:682:B:ILE:HG13 | 2:681:B:ILE:HD12 | 6        | 0.52          |
| (1,420)  | 2:682:B:ILE:HG13 | 2:681:B:ILE:HD13 | 6        | 0.52          |
| (1,359)  | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 6        | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,359)  | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 17       | 0.52          |
| (1,359)  | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 18       | 0.52          |
| (1,206)  | 2:686:B:ARG:HG2  | 2:653:B:ARG:HG2  | 1        | 0.52          |
| (1,197)  | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 10       | 0.52          |
| (1,182)  | 2:678:B:ALA:HB1  | 2:682:B:ILE:HG21 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB1  | 2:682:B:ILE:HG22 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB1  | 2:682:B:ILE:HG23 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB2  | 2:682:B:ILE:HG21 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB2  | 2:682:B:ILE:HG22 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB2  | 2:682:B:ILE:HG23 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB3  | 2:682:B:ILE:HG21 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB3  | 2:682:B:ILE:HG22 | 2        | 0.52          |
| (1,182)  | 2:678:B:ALA:HB3  | 2:682:B:ILE:HG23 | 2        | 0.52          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 6        | 0.52          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 6        | 0.52          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 6        | 0.52          |
| (1,106)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HG21 | 10       | 0.52          |
| (1,106)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HG22 | 10       | 0.52          |
| (1,106)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HG23 | 10       | 0.52          |
| (1,63)   | 2:630:B:THR:HA   | 2:634:B:LEU:HG   | 4        | 0.52          |
| (1,2749) | 1:221:A:ARG:HG3  | 1:221:A:ARG:H    | 17       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD11 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD12 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD11 | 1:220:A:LEU:HD13 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD11 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD12 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD12 | 1:220:A:LEU:HD13 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD11 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD12 | 20       | 0.51          |
| (1,2602) | 2:681:B:ILE:HD13 | 1:220:A:LEU:HD13 | 20       | 0.51          |
| (1,2058) | 2:645:B:SER:HB2  | 2:645:B:SER:H    | 10       | 0.51          |
| (1,1921) | 2:724:B:LYS:HG3  | 2:725:B:TYR:H    | 16       | 0.51          |
| (1,1812) | 2:712:B:ARG:HB2  | 2:712:B:ARG:H    | 8        | 0.51          |
| (1,1351) | 2:716:B:LYS:HE2  | 2:720:B:GLU:HG3  | 20       | 0.51          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 5        | 0.51          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 16       | 0.51          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 13       | 0.51          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 13       | 0.51          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 13       | 0.51          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 14       | 0.51          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 14       | 0.51          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 14       | 0.51          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,979) | 2:697:B:LEU:HA   | 2:700:B:LEU:HD21 | 8        | 0.51          |
| (1,979) | 2:697:B:LEU:HA   | 2:700:B:LEU:HD22 | 8        | 0.51          |
| (1,979) | 2:697:B:LEU:HA   | 2:700:B:LEU:HD23 | 8        | 0.51          |
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 1        | 0.51          |
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 1        | 0.51          |
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 1        | 0.51          |
| (1,688) | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 8        | 0.51          |
| (1,688) | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 8        | 0.51          |
| (1,688) | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 8        | 0.51          |
| (1,688) | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 12       | 0.51          |
| (1,688) | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 12       | 0.51          |
| (1,688) | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 12       | 0.51          |
| (1,688) | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 17       | 0.51          |
| (1,688) | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 17       | 0.51          |
| (1,688) | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 17       | 0.51          |
| (1,514) | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 16       | 0.51          |
| (1,514) | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 16       | 0.51          |
| (1,514) | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 16       | 0.51          |
| (1,466) | 2:726:B:TYR:HA   | 2:728:B:LYS:H    | 18       | 0.51          |
| (1,432) | 2:720:B:GLU:HB3  | 2:724:B:LYS:HE3  | 18       | 0.51          |
| (1,402) | 2:632:B:ARG:HG3  | 2:632:B:ARG:HD3  | 8        | 0.51          |
| (1,210) | 2:667:B:ARG:HB2  | 2:665:B:ILE:HG13 | 3        | 0.51          |
| (1,197) | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 5        | 0.51          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD21 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD22 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD23 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD21 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD22 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD23 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD21 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD22 | 9        | 0.51          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD23 | 9        | 0.51          |
| (1,179) | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG21 | 4        | 0.51          |
| (1,179) | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG22 | 4        | 0.51          |
| (1,179) | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG23 | 4        | 0.51          |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD21 | 6        | 0.51          |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD22 | 6        | 0.51          |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD23 | 6        | 0.51          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG11 | 20       | 0.51          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG12 | 20       | 0.51          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG13 | 20       | 0.51          |
| (1,19)  | 2:682:B:ILE:HG21 | 2:681:B:ILE:HA   | 8        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,19)   | 2:682:B:ILE:HG22 | 2:681:B:ILE:HA   | 8        | 0.51          |
| (1,19)   | 2:682:B:ILE:HG23 | 2:681:B:ILE:HA   | 8        | 0.51          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD21 | 5        | 0.5           |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD22 | 5        | 0.5           |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD23 | 5        | 0.5           |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 4        | 0.5           |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 4        | 0.5           |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 4        | 0.5           |
| (1,2058) | 2:645:B:SER:HB2  | 2:645:B:SER:H    | 3        | 0.5           |
| (1,2058) | 2:645:B:SER:HB2  | 2:645:B:SER:H    | 14       | 0.5           |
| (1,1423) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HG3  | 11       | 0.5           |
| (1,1423) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HG3  | 11       | 0.5           |
| (1,1423) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HG3  | 11       | 0.5           |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 4        | 0.5           |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 4        | 0.5           |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 4        | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 3        | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 3        | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 3        | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 8        | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 8        | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 8        | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 20       | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 20       | 0.5           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 20       | 0.5           |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD21 | 19       | 0.5           |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD22 | 19       | 0.5           |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD23 | 19       | 0.5           |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 15       | 0.5           |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 15       | 0.5           |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 15       | 0.5           |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 7        | 0.5           |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 7        | 0.5           |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 7        | 0.5           |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 14       | 0.5           |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 14       | 0.5           |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 14       | 0.5           |
| (1,574)  | 2:665:B:ILE:HD11 | 2:630:B:THR:H    | 1        | 0.5           |
| (1,574)  | 2:665:B:ILE:HD12 | 2:630:B:THR:H    | 1        | 0.5           |
| (1,574)  | 2:665:B:ILE:HD13 | 2:630:B:THR:H    | 1        | 0.5           |
| (1,535)  | 2:716:B:LYS:HD2  | 2:720:B:GLU:H    | 19       | 0.5           |
| (1,420)  | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD11 | 11       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,420)  | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD12 | 11       | 0.5           |
| (1,420)  | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD13 | 11       | 0.5           |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG21 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG22 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD21 | 2:673:B:ILE:HG23 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG21 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG22 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD22 | 2:673:B:ILE:HG23 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG21 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG22 | 8        | 0.5           |
| (1,418)  | 1:210:A:LEU:HD23 | 2:673:B:ILE:HG23 | 8        | 0.5           |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 20       | 0.5           |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 20       | 0.5           |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 4        | 0.5           |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 4        | 0.5           |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 4        | 0.5           |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 18       | 0.5           |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 18       | 0.5           |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 18       | 0.5           |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD21 | 17       | 0.49          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD22 | 17       | 0.49          |
| (1,2664) | 2:702:B:MET:HG2  | 1:211:A:LEU:HD23 | 17       | 0.49          |
| (1,2564) | 1:220:A:LEU:HD21 | 1:217:A:MET:HG3  | 8        | 0.49          |
| (1,2564) | 1:220:A:LEU:HD22 | 1:217:A:MET:HG3  | 8        | 0.49          |
| (1,2564) | 1:220:A:LEU:HD23 | 1:217:A:MET:HG3  | 8        | 0.49          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD21 | 20       | 0.49          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD22 | 20       | 0.49          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD23 | 20       | 0.49          |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 7        | 0.49          |
| (1,2413) | 2:699:B:ARG:HG3  | 2:699:B:ARG:H    | 20       | 0.49          |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 2        | 0.49          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 6        | 0.49          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 11       | 0.49          |
| (1,1406) | 2:693:B:VAL:HG11 | 2:689:B:PRO:HB2  | 13       | 0.49          |
| (1,1406) | 2:693:B:VAL:HG12 | 2:689:B:PRO:HB2  | 13       | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1406) | 2:693:B:VAL:HG13 | 2:689:B:PRO:HB2  | 13       | 0.49          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 7        | 0.49          |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 7        | 0.49          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 16       | 0.49          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 16       | 0.49          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 16       | 0.49          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 10       | 0.49          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 10       | 0.49          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 10       | 0.49          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 14       | 0.49          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 14       | 0.49          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 14       | 0.49          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 2        | 0.49          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 2        | 0.49          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 2        | 0.49          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 19       | 0.49          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 19       | 0.49          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 19       | 0.49          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 5        | 0.49          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 5        | 0.49          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 5        | 0.49          |
| (1,391)  | 2:728:B:LYS:HB3  | 2:728:B:LYS:HE3  | 18       | 0.49          |
| (1,304)  | 2:705:B:GLU:HA   | 2:708:B:ARG:HB3  | 10       | 0.49          |
| (1,282)  | 2:610:B:ILE:HD11 | 2:608:B:GLU:HG3  | 5        | 0.49          |
| (1,282)  | 2:610:B:ILE:HD12 | 2:608:B:GLU:HG3  | 5        | 0.49          |
| (1,282)  | 2:610:B:ILE:HD13 | 2:608:B:GLU:HG3  | 5        | 0.49          |
| (1,251)  | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB1  | 10       | 0.49          |
| (1,251)  | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB2  | 10       | 0.49          |
| (1,251)  | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB3  | 10       | 0.49          |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD11 | 7        | 0.49          |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD12 | 7        | 0.49          |
| (1,143)  | 2:634:B:LEU:HG   | 2:658:B:LEU:HD13 | 7        | 0.49          |
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 14       | 0.49          |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 14       | 0.49          |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 14       | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 19       | 0.49          |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 19       | 0.49          |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 19       | 0.49          |
| (2,14)   | 1:220:A:LEU:HD21 | 1:217:A:MET:HG2  | 9        | 0.48          |
| (2,14)   | 1:220:A:LEU:HD22 | 1:217:A:MET:HG2  | 9        | 0.48          |
| (2,14)   | 1:220:A:LEU:HD23 | 1:217:A:MET:HG2  | 9        | 0.48          |
| (2,1)    | 2:655:B:ASP:HB2  | 2:656:B:ASN:HA   | 10       | 0.48          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD21 | 19       | 0.48          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD22 | 19       | 0.48          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD23 | 19       | 0.48          |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 5        | 0.48          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 6        | 0.48          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 6        | 0.48          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 6        | 0.48          |
| (1,998)  | 2:695:B:ILE:HA   | 2:698:B:LYS:HD2  | 20       | 0.48          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 7        | 0.48          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 7        | 0.48          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 7        | 0.48          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 6        | 0.48          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 6        | 0.48          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 6        | 0.48          |
| (1,697)  | 2:687:B:LYS:HD2  | 2:688:B:ASN:H    | 17       | 0.48          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 2        | 0.48          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 2        | 0.48          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 2        | 0.48          |
| (1,535)  | 2:716:B:LYS:HD2  | 2:720:B:GLU:H    | 14       | 0.48          |
| (1,528)  | 2:611:B:TYR:HB2  | 2:611:B:TYR:H    | 15       | 0.48          |
| (1,414)  | 2:672:B:ARG:HG2  | 2:673:B:ILE:HG21 | 11       | 0.48          |
| (1,414)  | 2:672:B:ARG:HG2  | 2:673:B:ILE:HG22 | 11       | 0.48          |
| (1,414)  | 2:672:B:ARG:HG2  | 2:673:B:ILE:HG23 | 11       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB1  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB2  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB3  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB1  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB2  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB3  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB1  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB2  | 16       | 0.48          |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB3  | 16       | 0.48          |
| (1,281)  | 2:622:B:VAL:HG11 | 2:619:B:GLU:HG3  | 6        | 0.48          |
| (1,281)  | 2:622:B:VAL:HG12 | 2:619:B:GLU:HG3  | 6        | 0.48          |
| (1,281)  | 2:622:B:VAL:HG13 | 2:619:B:GLU:HG3  | 6        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,278)  | 2:670:B:LEU:HD21 | 2:696:B:VAL:HB   | 2        | 0.48          |
| (1,278)  | 2:670:B:LEU:HD22 | 2:696:B:VAL:HB   | 2        | 0.48          |
| (1,278)  | 2:670:B:LEU:HD23 | 2:696:B:VAL:HB   | 2        | 0.48          |
| (1,272)  | 2:628:B:LEU:HD11 | 2:632:B:ARG:HB3  | 8        | 0.48          |
| (1,272)  | 2:628:B:LEU:HD12 | 2:632:B:ARG:HB3  | 8        | 0.48          |
| (1,272)  | 2:628:B:LEU:HD13 | 2:632:B:ARG:HB3  | 8        | 0.48          |
| (1,266)  | 2:658:B:LEU:HD11 | 2:634:B:LEU:HG   | 9        | 0.48          |
| (1,266)  | 2:658:B:LEU:HD12 | 2:634:B:LEU:HG   | 9        | 0.48          |
| (1,266)  | 2:658:B:LEU:HD13 | 2:634:B:LEU:HG   | 9        | 0.48          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 3        | 0.48          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 3        | 0.48          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 3        | 0.48          |
| (1,197)  | 2:641:B:LEU:HD11 | 2:649:B:GLN:HA   | 18       | 0.48          |
| (1,197)  | 2:641:B:LEU:HD12 | 2:649:B:GLN:HA   | 18       | 0.48          |
| (1,197)  | 2:641:B:LEU:HD13 | 2:649:B:GLN:HA   | 18       | 0.48          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD11 | 10       | 0.48          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD12 | 10       | 0.48          |
| (1,143)  | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD13 | 10       | 0.48          |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD11 | 16       | 0.47          |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD12 | 16       | 0.47          |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD13 | 16       | 0.47          |
| (1,2463) | 2:621:B:ASP:HA   | 2:711:B:GLN:HE22 | 4        | 0.47          |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 7        | 0.47          |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 7        | 0.47          |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 7        | 0.47          |
| (1,1892) | 2:612:B:ARG:HG2  | 2:612:B:ARG:H    | 10       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD11 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD12 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD11 | 2:700:B:LEU:HD13 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD11 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD12 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD12 | 2:700:B:LEU:HD13 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD11 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD12 | 14       | 0.47          |
| (1,1226) | 2:673:B:ILE:HD13 | 2:700:B:LEU:HD13 | 14       | 0.47          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 7        | 0.47          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 7        | 0.47          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 7        | 0.47          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 10       | 0.47          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 10       | 0.47          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 10       | 0.47          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD21 | 10       | 0.47          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,951) | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD22 | 10       | 0.47          |
| (1,951) | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD23 | 10       | 0.47          |
| (1,939) | 2:639:B:LYS:HA   | 2:639:B:LYS:HG3  | 11       | 0.47          |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 14       | 0.47          |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 14       | 0.47          |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 14       | 0.47          |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 5        | 0.47          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 5        | 0.47          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 5        | 0.47          |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 15       | 0.47          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 15       | 0.47          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 15       | 0.47          |
| (1,574) | 2:631:B:ILE:HG21 | 2:630:B:THR:H    | 15       | 0.47          |
| (1,574) | 2:631:B:ILE:HG22 | 2:630:B:THR:H    | 15       | 0.47          |
| (1,574) | 2:631:B:ILE:HG23 | 2:630:B:THR:H    | 15       | 0.47          |
| (1,433) | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 17       | 0.47          |
| (1,429) | 2:717:B:VAL:HA   | 2:716:B:LYS:HD2  | 2        | 0.47          |
| (1,389) | 2:677:B:LYS:HG2  | 2:677:B:LYS:HE2  | 18       | 0.47          |
| (1,384) | 2:693:B:VAL:HG21 | 2:694:B:PRO:HA   | 15       | 0.47          |
| (1,384) | 2:693:B:VAL:HG22 | 2:694:B:PRO:HA   | 15       | 0.47          |
| (1,384) | 2:693:B:VAL:HG23 | 2:694:B:PRO:HA   | 15       | 0.47          |
| (1,359) | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 10       | 0.47          |
| (1,266) | 2:631:B:ILE:HD11 | 2:634:B:LEU:HG   | 4        | 0.47          |
| (1,266) | 2:631:B:ILE:HD12 | 2:634:B:LEU:HG   | 4        | 0.47          |
| (1,266) | 2:631:B:ILE:HD13 | 2:634:B:LEU:HG   | 4        | 0.47          |
| (1,260) | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 6        | 0.47          |
| (1,260) | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 6        | 0.47          |
| (1,260) | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 6        | 0.47          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB1  | 5        | 0.47          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB2  | 5        | 0.47          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB3  | 5        | 0.47          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 20       | 0.47          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 20       | 0.47          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 20       | 0.47          |
| (1,178) | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD11 | 14       | 0.47          |
| (1,178) | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD12 | 14       | 0.47          |
| (1,178) | 2:700:B:LEU:HD11 | 2:673:B:ILE:HD13 | 14       | 0.47          |
| (1,178) | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD11 | 14       | 0.47          |
| (1,178) | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD12 | 14       | 0.47          |
| (1,178) | 2:700:B:LEU:HD12 | 2:673:B:ILE:HD13 | 14       | 0.47          |
| (1,178) | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD11 | 14       | 0.47          |
| (1,178) | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD12 | 14       | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,178)  | 2:700:B:LEU:HD13 | 2:673:B:ILE:HD13 | 14       | 0.47          |
| (1,158)  | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG11 | 13       | 0.47          |
| (1,158)  | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG12 | 13       | 0.47          |
| (1,158)  | 2:641:B:LEU:HB3  | 2:693:B:VAL:HG13 | 13       | 0.47          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 5        | 0.47          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 5        | 0.47          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 5        | 0.47          |
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 4        | 0.47          |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 4        | 0.47          |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 4        | 0.47          |
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 6        | 0.47          |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 6        | 0.47          |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 6        | 0.47          |
| (1,19)   | 2:682:B:ILE:HG21 | 2:681:B:ILE:HA   | 13       | 0.47          |
| (1,19)   | 2:682:B:ILE:HG22 | 2:681:B:ILE:HA   | 13       | 0.47          |
| (1,19)   | 2:682:B:ILE:HG23 | 2:681:B:ILE:HA   | 13       | 0.47          |
| (1,15)   | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD3  | 10       | 0.47          |
| (1,15)   | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD3  | 10       | 0.47          |
| (1,15)   | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD3  | 10       | 0.47          |
| (1,2557) | 1:220:A:LEU:HD21 | 1:217:A:MET:HA   | 16       | 0.46          |
| (1,2557) | 1:220:A:LEU:HD22 | 1:217:A:MET:HA   | 16       | 0.46          |
| (1,2557) | 1:220:A:LEU:HD23 | 1:217:A:MET:HA   | 16       | 0.46          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD21 | 5        | 0.46          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD22 | 5        | 0.46          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD23 | 5        | 0.46          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD21 | 5        | 0.46          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD22 | 5        | 0.46          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD23 | 5        | 0.46          |
| (1,2413) | 2:699:B:ARG:HG3  | 2:699:B:ARG:H    | 5        | 0.46          |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 4        | 0.46          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 14       | 0.46          |
| (1,1418) | 2:717:B:VAL:HG11 | 2:720:B:GLU:HG2  | 3        | 0.46          |
| (1,1418) | 2:717:B:VAL:HG12 | 2:720:B:GLU:HG2  | 3        | 0.46          |
| (1,1418) | 2:717:B:VAL:HG13 | 2:720:B:GLU:HG2  | 3        | 0.46          |
| (1,938)  | 2:720:B:GLU:HA   | 2:724:B:LYS:HG3  | 5        | 0.46          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 6        | 0.46          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 6        | 0.46          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 6        | 0.46          |
| (1,740)  | 2:704:B:GLU:HG3  | 2:704:B:GLU:H    | 7        | 0.46          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 8        | 0.46          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 9        | 0.46          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 12       | 0.46          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 11       | 0.46          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 11       | 0.46          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 11       | 0.46          |
| (1,464) | 2:647:B:GLU:HA   | 2:649:B:GLN:HE21 | 11       | 0.46          |
| (1,464) | 2:645:B:SER:HB2  | 2:649:B:GLN:HE21 | 14       | 0.46          |
| (1,432) | 2:700:B:LEU:HG   | 2:701:B:LYS:HE2  | 15       | 0.46          |
| (1,409) | 2:620:B:LEU:HD11 | 2:711:B:GLN:HA   | 6        | 0.46          |
| (1,409) | 2:620:B:LEU:HD12 | 2:711:B:GLN:HA   | 6        | 0.46          |
| (1,409) | 2:620:B:LEU:HD13 | 2:711:B:GLN:HA   | 6        | 0.46          |
| (1,408) | 2:697:B:LEU:HD21 | 2:697:B:LEU:HA   | 7        | 0.46          |
| (1,408) | 2:697:B:LEU:HD22 | 2:697:B:LEU:HA   | 7        | 0.46          |
| (1,408) | 2:697:B:LEU:HD23 | 2:697:B:LEU:HA   | 7        | 0.46          |
| (1,384) | 2:693:B:VAL:HG21 | 2:694:B:PRO:HA   | 19       | 0.46          |
| (1,384) | 2:693:B:VAL:HG22 | 2:694:B:PRO:HA   | 19       | 0.46          |
| (1,384) | 2:693:B:VAL:HG23 | 2:694:B:PRO:HA   | 19       | 0.46          |
| (1,282) | 2:610:B:ILE:HD11 | 2:608:B:GLU:HG3  | 11       | 0.46          |
| (1,282) | 2:610:B:ILE:HD12 | 2:608:B:GLU:HG3  | 11       | 0.46          |
| (1,282) | 2:610:B:ILE:HD13 | 2:608:B:GLU:HG3  | 11       | 0.46          |
| (1,256) | 2:658:B:LEU:HD11 | 2:630:B:THR:HG21 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD11 | 2:630:B:THR:HG22 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD11 | 2:630:B:THR:HG23 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD12 | 2:630:B:THR:HG21 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD12 | 2:630:B:THR:HG22 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD12 | 2:630:B:THR:HG23 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD13 | 2:630:B:THR:HG21 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD13 | 2:630:B:THR:HG22 | 16       | 0.46          |
| (1,256) | 2:658:B:LEU:HD13 | 2:630:B:THR:HG23 | 16       | 0.46          |
| (1,248) | 2:703:B:LYS:HG2  | 2:702:B:MET:HE1  | 2        | 0.46          |
| (1,248) | 2:703:B:LYS:HG2  | 2:702:B:MET:HE2  | 2        | 0.46          |
| (1,248) | 2:703:B:LYS:HG2  | 2:702:B:MET:HE3  | 2        | 0.46          |
| (1,214) | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 15       | 0.46          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 9        | 0.46          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 9        | 0.46          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 9        | 0.46          |
| (1,106) | 2:662:B:SER:HB3  | 2:665:B:ILE:HG21 | 19       | 0.46          |
| (1,106) | 2:662:B:SER:HB3  | 2:665:B:ILE:HG22 | 19       | 0.46          |
| (1,106) | 2:662:B:SER:HB3  | 2:665:B:ILE:HG23 | 19       | 0.46          |
| (1,19)  | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 11       | 0.46          |
| (1,19)  | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 11       | 0.46          |
| (1,19)  | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 11       | 0.46          |
| (1,18)  | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE3  | 4        | 0.46          |
| (1,18)  | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE3  | 4        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,18)   | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE3  | 4        | 0.46          |
| (1,2718) | 1:215:A:GLN:HG2  | 1:215:A:GLN:H    | 10       | 0.45          |
| (1,2413) | 2:699:B:ARG:HG3  | 2:699:B:ARG:H    | 13       | 0.45          |
| (1,2219) | 1:220:A:LEU:HD11 | 2:680:B:ASP:H    | 9        | 0.45          |
| (1,2219) | 1:220:A:LEU:HD12 | 2:680:B:ASP:H    | 9        | 0.45          |
| (1,2219) | 1:220:A:LEU:HD13 | 2:680:B:ASP:H    | 9        | 0.45          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 18       | 0.45          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 16       | 0.45          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 1        | 0.45          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD11 | 4        | 0.45          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD12 | 4        | 0.45          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD13 | 4        | 0.45          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD11 | 4        | 0.45          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD12 | 4        | 0.45          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD13 | 4        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD21 | 2:693:B:VAL:HG11 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD21 | 2:693:B:VAL:HG12 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD21 | 2:693:B:VAL:HG13 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD22 | 2:693:B:VAL:HG11 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD22 | 2:693:B:VAL:HG12 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD22 | 2:693:B:VAL:HG13 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD23 | 2:693:B:VAL:HG11 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD23 | 2:693:B:VAL:HG12 | 7        | 0.45          |
| (1,1244) | 2:685:B:LEU:HD23 | 2:693:B:VAL:HG13 | 7        | 0.45          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 5        | 0.45          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 5        | 0.45          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 5        | 0.45          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 3        | 0.45          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 3        | 0.45          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 3        | 0.45          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD11 | 12       | 0.45          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD12 | 12       | 0.45          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD13 | 12       | 0.45          |
| (1,740)  | 2:704:B:GLU:HG3  | 2:704:B:GLU:H    | 3        | 0.45          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 11       | 0.45          |
| (1,740)  | 2:704:B:GLU:HG3  | 2:704:B:GLU:H    | 14       | 0.45          |
| (1,619)  | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 8        | 0.45          |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 11       | 0.45          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 1        | 0.45          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 1        | 0.45          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 1        | 0.45          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 13       | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 13       | 0.45          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 13       | 0.45          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 17       | 0.45          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 17       | 0.45          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 17       | 0.45          |
| (1,499)  | 2:620:B:LEU:HB2  | 2:622:B:VAL:H    | 2        | 0.45          |
| (1,444)  | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD21 | 3        | 0.45          |
| (1,444)  | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD22 | 3        | 0.45          |
| (1,444)  | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD23 | 3        | 0.45          |
| (1,429)  | 2:717:B:VAL:HA   | 2:716:B:LYS:HD2  | 19       | 0.45          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 3        | 0.45          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 3        | 0.45          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 3        | 0.45          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 18       | 0.45          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 18       | 0.45          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 18       | 0.45          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 6        | 0.45          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 6        | 0.45          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 6        | 0.45          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD21 | 6        | 0.45          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD22 | 6        | 0.45          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD23 | 6        | 0.45          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG11 | 7        | 0.44          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG12 | 7        | 0.44          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG13 | 7        | 0.44          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD21 | 20       | 0.44          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD22 | 20       | 0.44          |
| (1,2663) | 2:703:B:LYS:HE2  | 1:211:A:LEU:HD23 | 20       | 0.44          |
| (1,2557) | 1:220:A:LEU:HD21 | 1:217:A:MET:HA   | 20       | 0.44          |
| (1,2557) | 1:220:A:LEU:HD22 | 1:217:A:MET:HA   | 20       | 0.44          |
| (1,2557) | 1:220:A:LEU:HD23 | 1:217:A:MET:HA   | 20       | 0.44          |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 17       | 0.44          |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG3  | 1        | 0.44          |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG3  | 19       | 0.44          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD21 | 4        | 0.44          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD22 | 4        | 0.44          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD23 | 4        | 0.44          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 6        | 0.44          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 6        | 0.44          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 6        | 0.44          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 4        | 0.44          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 5        | 0.44          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,740) | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 15       | 0.44          |
| (1,667) | 1:220:A:LEU:HD21 | 2:677:B:LYS:H    | 20       | 0.44          |
| (1,667) | 1:220:A:LEU:HD22 | 2:677:B:LYS:H    | 20       | 0.44          |
| (1,667) | 1:220:A:LEU:HD23 | 2:677:B:LYS:H    | 20       | 0.44          |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 10       | 0.44          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 10       | 0.44          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 10       | 0.44          |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 20       | 0.44          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 20       | 0.44          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 20       | 0.44          |
| (1,535) | 2:716:B:LYS:HD3  | 2:720:B:GLU:H    | 11       | 0.44          |
| (1,521) | 2:677:B:LYS:HG3  | 2:677:B:LYS:H    | 2        | 0.44          |
| (1,499) | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 9        | 0.44          |
| (1,477) | 2:712:B:ARG:HA   | 2:715:B:ASN:H    | 5        | 0.44          |
| (1,441) | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG21 | 6        | 0.44          |
| (1,441) | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG22 | 6        | 0.44          |
| (1,441) | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG23 | 6        | 0.44          |
| (1,289) | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 1        | 0.44          |
| (1,289) | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 1        | 0.44          |
| (1,289) | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 1        | 0.44          |
| (1,278) | 2:670:B:LEU:HD21 | 2:696:B:VAL:HB   | 17       | 0.44          |
| (1,278) | 2:670:B:LEU:HD22 | 2:696:B:VAL:HB   | 17       | 0.44          |
| (1,278) | 2:670:B:LEU:HD23 | 2:696:B:VAL:HB   | 17       | 0.44          |
| (1,272) | 2:628:B:LEU:HD11 | 2:632:B:ARG:HB3  | 20       | 0.44          |
| (1,272) | 2:628:B:LEU:HD12 | 2:632:B:ARG:HB3  | 20       | 0.44          |
| (1,272) | 2:628:B:LEU:HD13 | 2:632:B:ARG:HB3  | 20       | 0.44          |
| (1,248) | 2:703:B:LYS:HG2  | 2:702:B:MET:HE1  | 8        | 0.44          |
| (1,248) | 2:703:B:LYS:HG2  | 2:702:B:MET:HE2  | 8        | 0.44          |
| (1,248) | 2:703:B:LYS:HG2  | 2:702:B:MET:HE3  | 8        | 0.44          |
| (1,133) | 2:648:B:GLU:HG2  | 2:644:B:LEU:HD11 | 10       | 0.44          |
| (1,133) | 2:648:B:GLU:HG2  | 2:644:B:LEU:HD12 | 10       | 0.44          |
| (1,133) | 2:648:B:GLU:HG2  | 2:644:B:LEU:HD13 | 10       | 0.44          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD11 | 13       | 0.44          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD12 | 13       | 0.44          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD13 | 13       | 0.44          |
| (1,49)  | 2:649:B:GLN:HA   | 2:644:B:LEU:HD21 | 11       | 0.44          |
| (1,49)  | 2:649:B:GLN:HA   | 2:644:B:LEU:HD22 | 11       | 0.44          |
| (1,49)  | 2:649:B:GLN:HA   | 2:644:B:LEU:HD23 | 11       | 0.44          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 15       | 0.44          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 15       | 0.44          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 15       | 0.44          |
| (1,30)  | 2:628:B:LEU:HA   | 2:700:B:LEU:HD11 | 6        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,30)   | 2:628:B:LEU:HA   | 2:700:B:LEU:HD12 | 6        | 0.44          |
| (1,30)   | 2:628:B:LEU:HA   | 2:700:B:LEU:HD13 | 6        | 0.44          |
| (1,12)   | 2:718:B:TRP:HZ3  | 2:723:B:GLU:HA   | 12       | 0.44          |
| (1,2710) | 1:213:A:ASP:HB2  | 1:214:A:GLU:H    | 9        | 0.43          |
| (1,2413) | 2:699:B:ARG:HG3  | 2:699:B:ARG:H    | 19       | 0.43          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 1        | 0.43          |
| (1,1892) | 2:612:B:ARG:HG2  | 2:612:B:ARG:H    | 1        | 0.43          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 6        | 0.43          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 15       | 0.43          |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 6        | 0.43          |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG11 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG12 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG13 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG11 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG12 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG13 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG11 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG12 | 16       | 0.43          |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG13 | 16       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD11 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD12 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD13 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD11 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD12 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD13 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD11 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD12 | 19       | 0.43          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD13 | 19       | 0.43          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 4        | 0.43          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 4        | 0.43          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 4        | 0.43          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 6        | 0.43          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 13       | 0.43          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 13       | 0.43          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 13       | 0.43          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 13       | 0.43          |
| (1,466)  | 2:726:B:TYR:HA   | 2:728:B:LYS:H    | 10       | 0.43          |
| (1,456)  | 1:226:A:LEU:HB3  | 2:688:B:ASN:HD21 | 5        | 0.43          |
| (1,433)  | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 11       | 0.43          |
| (1,384)  | 2:693:B:VAL:HG21 | 2:694:B:PRO:HA   | 9        | 0.43          |
| (1,384)  | 2:693:B:VAL:HG22 | 2:694:B:PRO:HA   | 9        | 0.43          |
| (1,384)  | 2:693:B:VAL:HG23 | 2:694:B:PRO:HA   | 9        | 0.43          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,359) | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 20       | 0.43          |
| (1,354) | 2:715:B:ASN:HB3  | 2:712:B:ARG:HA   | 5        | 0.43          |
| (1,289) | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB2  | 7        | 0.43          |
| (1,289) | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB2  | 7        | 0.43          |
| (1,289) | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB2  | 7        | 0.43          |
| (1,289) | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 16       | 0.43          |
| (1,289) | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 16       | 0.43          |
| (1,289) | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 16       | 0.43          |
| (1,271) | 2:644:B:LEU:HD21 | 2:651:B:LYS:HD3  | 1        | 0.43          |
| (1,271) | 2:644:B:LEU:HD22 | 2:651:B:LYS:HD3  | 1        | 0.43          |
| (1,271) | 2:644:B:LEU:HD23 | 2:651:B:LYS:HD3  | 1        | 0.43          |
| (1,265) | 2:697:B:LEU:HD21 | 2:638:B:GLN:HB2  | 12       | 0.43          |
| (1,265) | 2:697:B:LEU:HD22 | 2:638:B:GLN:HB2  | 12       | 0.43          |
| (1,265) | 2:697:B:LEU:HD23 | 2:638:B:GLN:HB2  | 12       | 0.43          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 8        | 0.43          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 8        | 0.43          |
| (1,251) | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 8        | 0.43          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD11 | 12       | 0.43          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD12 | 12       | 0.43          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD13 | 12       | 0.43          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG21 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG22 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG23 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG21 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG22 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG23 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG21 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG22 | 15       | 0.43          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG23 | 15       | 0.43          |
| (1,179) | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 5        | 0.43          |
| (1,179) | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 5        | 0.43          |
| (1,179) | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 5        | 0.43          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 3        | 0.43          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 3        | 0.43          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 3        | 0.43          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 17       | 0.43          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 17       | 0.43          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 17       | 0.43          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG21 | 4        | 0.43          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG22 | 4        | 0.43          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG23 | 4        | 0.43          |
| (1,74)  | 2:613:B:CYS:HB3  | 2:612:B:ARG:HB2  | 9        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 10       | 0.43          |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 10       | 0.43          |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 10       | 0.43          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:667:B:ARG:HD3  | 13       | 0.43          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:667:B:ARG:HD3  | 13       | 0.43          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:667:B:ARG:HD3  | 13       | 0.43          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD2  | 14       | 0.43          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD2  | 14       | 0.43          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD2  | 14       | 0.43          |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 14       | 0.42          |
| (1,2112) | 2:644:B:LEU:HD21 | 2:652:B:PHE:H    | 2        | 0.42          |
| (1,2112) | 2:644:B:LEU:HD22 | 2:652:B:PHE:H    | 2        | 0.42          |
| (1,2112) | 2:644:B:LEU:HD23 | 2:652:B:PHE:H    | 2        | 0.42          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 7        | 0.42          |
| (1,1873) | 2:608:B:GLU:HB2  | 2:608:B:GLU:H    | 6        | 0.42          |
| (1,1570) | 2:647:B:GLU:HG3  | 2:647:B:GLU:HA   | 18       | 0.42          |
| (1,1200) | 2:658:B:LEU:HG   | 2:637:B:ILE:HD11 | 5        | 0.42          |
| (1,1200) | 2:658:B:LEU:HG   | 2:637:B:ILE:HD12 | 5        | 0.42          |
| (1,1200) | 2:658:B:LEU:HG   | 2:637:B:ILE:HD13 | 5        | 0.42          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 2        | 0.42          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 2        | 0.42          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 2        | 0.42          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 5        | 0.42          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 5        | 0.42          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 5        | 0.42          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 19       | 0.42          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 19       | 0.42          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 19       | 0.42          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD21 | 12       | 0.42          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD22 | 12       | 0.42          |
| (1,765)  | 2:676:B:ASP:HB2  | 1:210:A:LEU:HD23 | 12       | 0.42          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD21 | 12       | 0.42          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD22 | 12       | 0.42          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD23 | 12       | 0.42          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 12       | 0.42          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 16       | 0.42          |
| (1,688)  | 2:670:B:LEU:HD11 | 2:685:B:LEU:H    | 11       | 0.42          |
| (1,688)  | 2:670:B:LEU:HD12 | 2:685:B:LEU:H    | 11       | 0.42          |
| (1,688)  | 2:670:B:LEU:HD13 | 2:685:B:LEU:H    | 11       | 0.42          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 14       | 0.42          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 14       | 0.42          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 14       | 0.42          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,672) | 2:677:B:LYS:HD2  | 2:678:B:ALA:H    | 12       | 0.42          |
| (1,672) | 2:677:B:LYS:HD2  | 2:678:B:ALA:H    | 15       | 0.42          |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 18       | 0.42          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 18       | 0.42          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 18       | 0.42          |
| (1,441) | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG21 | 15       | 0.42          |
| (1,441) | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG22 | 15       | 0.42          |
| (1,441) | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG23 | 15       | 0.42          |
| (1,440) | 2:693:B:VAL:HG21 | 2:638:B:GLN:HG3  | 13       | 0.42          |
| (1,440) | 2:693:B:VAL:HG22 | 2:638:B:GLN:HG3  | 13       | 0.42          |
| (1,440) | 2:693:B:VAL:HG23 | 2:638:B:GLN:HG3  | 13       | 0.42          |
| (1,420) | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD11 | 5        | 0.42          |
| (1,420) | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD12 | 5        | 0.42          |
| (1,420) | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD13 | 5        | 0.42          |
| (1,355) | 2:712:B:ARG:HG3  | 2:712:B:ARG:HA   | 8        | 0.42          |
| (1,279) | 2:697:B:LEU:HD11 | 2:638:B:GLN:HG3  | 5        | 0.42          |
| (1,279) | 2:697:B:LEU:HD12 | 2:638:B:GLN:HG3  | 5        | 0.42          |
| (1,279) | 2:697:B:LEU:HD13 | 2:638:B:GLN:HG3  | 5        | 0.42          |
| (1,278) | 2:685:B:LEU:HD11 | 2:696:B:VAL:HB   | 8        | 0.42          |
| (1,278) | 2:685:B:LEU:HD12 | 2:696:B:VAL:HB   | 8        | 0.42          |
| (1,278) | 2:685:B:LEU:HD13 | 2:696:B:VAL:HB   | 8        | 0.42          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB1  | 19       | 0.42          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB2  | 19       | 0.42          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB3  | 19       | 0.42          |
| (1,210) | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 11       | 0.42          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 13       | 0.42          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 13       | 0.42          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 13       | 0.42          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 13       | 0.42          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 13       | 0.42          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 13       | 0.42          |
| (1,192) | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD11 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD12 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD11 | 2:670:B:LEU:HD13 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD11 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD12 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD12 | 2:670:B:LEU:HD13 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD11 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD12 | 12       | 0.42          |
| (1,192) | 2:673:B:ILE:HD13 | 2:670:B:LEU:HD13 | 12       | 0.42          |
| (1,183) | 2:685:B:LEU:HG   | 2:682:B:ILE:HG21 | 7        | 0.42          |
| (1,183) | 2:685:B:LEU:HG   | 2:682:B:ILE:HG22 | 7        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,183)  | 2:685:B:LEU:HG   | 2:682:B:ILE:HG23 | 7        | 0.42          |
| (1,151)  | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD11 | 16       | 0.42          |
| (1,151)  | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD12 | 16       | 0.42          |
| (1,151)  | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD13 | 16       | 0.42          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 18       | 0.42          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 18       | 0.42          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 18       | 0.42          |
| (1,88)   | 2:647:B:GLU:HA   | 2:647:B:GLU:HG3  | 18       | 0.42          |
| (1,61)   | 2:632:B:ARG:HA   | 2:632:B:ARG:HG3  | 2        | 0.42          |
| (1,16)   | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD3  | 8        | 0.42          |
| (1,16)   | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD3  | 8        | 0.42          |
| (1,16)   | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD3  | 8        | 0.42          |
| (1,2710) | 1:213:A:ASP:HB3  | 1:214:A:GLU:H    | 18       | 0.41          |
| (1,2672) | 1:206:A:GLN:HB2  | 1:206:A:GLN:H    | 11       | 0.41          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD21 | 3        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD22 | 3        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD23 | 3        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD21 | 3        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD22 | 3        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD23 | 3        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD21 | 8        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD22 | 8        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD23 | 8        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD21 | 8        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD22 | 8        | 0.41          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD23 | 8        | 0.41          |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 10       | 0.41          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 9        | 0.41          |
| (1,1852) | 2:701:B:LYS:HD2  | 2:700:B:LEU:H    | 1        | 0.41          |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 9        | 0.41          |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 15       | 0.41          |
| (1,1710) | 2:625:B:GLU:HA   | 2:625:B:GLU:HG3  | 6        | 0.41          |
| (1,1680) | 2:708:B:ARG:HB3  | 2:708:B:ARG:HD2  | 5        | 0.41          |
| (1,1680) | 2:708:B:ARG:HB3  | 2:708:B:ARG:HD2  | 16       | 0.41          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG3  | 8        | 0.41          |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 5        | 0.41          |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 19       | 0.41          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 15       | 0.41          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 15       | 0.41          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 15       | 0.41          |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG21 | 16       | 0.41          |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG22 | 16       | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG23 | 16       | 0.41          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD21 | 13       | 0.41          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD22 | 13       | 0.41          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD23 | 13       | 0.41          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 4        | 0.41          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 4        | 0.41          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 4        | 0.41          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 13       | 0.41          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 13       | 0.41          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 17       | 0.41          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 18       | 0.41          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 19       | 0.41          |
| (1,702)  | 2:691:B:ILE:HD11 | 2:690:B:SER:H    | 7        | 0.41          |
| (1,702)  | 2:691:B:ILE:HD12 | 2:690:B:SER:H    | 7        | 0.41          |
| (1,702)  | 2:691:B:ILE:HD13 | 2:690:B:SER:H    | 7        | 0.41          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 20       | 0.41          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 20       | 0.41          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 20       | 0.41          |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 8        | 0.41          |
| (1,672)  | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 11       | 0.41          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 16       | 0.41          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 16       | 0.41          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 16       | 0.41          |
| (1,441)  | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG21 | 9        | 0.41          |
| (1,441)  | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG22 | 9        | 0.41          |
| (1,441)  | 2:684:B:GLY:HA3  | 2:696:B:VAL:HG23 | 9        | 0.41          |
| (1,408)  | 2:634:B:LEU:HD11 | 2:697:B:LEU:HA   | 2        | 0.41          |
| (1,408)  | 2:634:B:LEU:HD12 | 2:697:B:LEU:HA   | 2        | 0.41          |
| (1,408)  | 2:634:B:LEU:HD13 | 2:697:B:LEU:HA   | 2        | 0.41          |
| (1,316)  | 2:629:B:ALA:HA   | 2:632:B:ARG:HD2  | 1        | 0.41          |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 16       | 0.41          |
| (1,300)  | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 16       | 0.41          |
| (1,251)  | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB1  | 14       | 0.41          |
| (1,251)  | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB2  | 14       | 0.41          |
| (1,251)  | 2:632:B:ARG:HB2  | 2:629:B:ALA:HB3  | 14       | 0.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,197) | 2:644:B:LEU:HD21 | 2:649:B:GLN:HA   | 4        | 0.41          |
| (1,197) | 2:644:B:LEU:HD22 | 2:649:B:GLN:HA   | 4        | 0.41          |
| (1,197) | 2:644:B:LEU:HD23 | 2:649:B:GLN:HA   | 4        | 0.41          |
| (1,197) | 2:644:B:LEU:HD21 | 2:649:B:GLN:HA   | 15       | 0.41          |
| (1,197) | 2:644:B:LEU:HD22 | 2:649:B:GLN:HA   | 15       | 0.41          |
| (1,197) | 2:644:B:LEU:HD23 | 2:649:B:GLN:HA   | 15       | 0.41          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 4        | 0.41          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 4        | 0.41          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 2        | 0.41          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 2        | 0.41          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 2        | 0.41          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 6        | 0.41          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 6        | 0.41          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 6        | 0.41          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 18       | 0.41          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 18       | 0.41          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 18       | 0.41          |
| (1,66)  | 2:687:B:LYS:HA   | 2:687:B:LYS:HD3  | 1        | 0.41          |
| (1,66)  | 2:636:B:ALA:HA   | 2:639:B:LYS:HD3  | 9        | 0.41          |
| (1,61)  | 2:632:B:ARG:HA   | 2:632:B:ARG:HG3  | 12       | 0.41          |
| (1,19)  | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 1        | 0.41          |
| (1,19)  | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 1        | 0.41          |
| (1,19)  | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 1        | 0.41          |
| (1,14)  | 2:658:B:LEU:HD11 | 2:686:B:ARG:HD2  | 7        | 0.41          |
| (1,14)  | 2:658:B:LEU:HD12 | 2:686:B:ARG:HD2  | 7        | 0.41          |
| (1,14)  | 2:658:B:LEU:HD13 | 2:686:B:ARG:HD2  | 7        | 0.41          |
| (2,13)  | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD21 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD22 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD23 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD21 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD22 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD23 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD21 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD22 | 1        | 0.4           |
| (2,13)  | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD23 | 1        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2710) | 1:213:A:ASP:HB2  | 1:214:A:GLU:H    | 1        | 0.4           |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 7        | 0.4           |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 7        | 0.4           |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 7        | 0.4           |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 10       | 0.4           |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 10       | 0.4           |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 10       | 0.4           |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 10       | 0.4           |
| (1,2019) | 2:682:B:ILE:HG12 | 2:682:B:ILE:H    | 3        | 0.4           |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG3  | 17       | 0.4           |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG3  | 18       | 0.4           |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 8        | 0.4           |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 8        | 0.4           |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE3  | 13       | 0.4           |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE3  | 13       | 0.4           |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE3  | 13       | 0.4           |
| (1,1570) | 2:647:B:GLU:HG2  | 2:647:B:GLU:HA   | 1        | 0.4           |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 10       | 0.4           |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 11       | 0.4           |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG3  | 12       | 0.4           |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 3        | 0.4           |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 20       | 0.4           |
| (1,1276) | 2:654:B:LEU:HD21 | 2:686:B:ARG:HA   | 1        | 0.4           |
| (1,1276) | 2:654:B:LEU:HD22 | 2:686:B:ARG:HA   | 1        | 0.4           |
| (1,1276) | 2:654:B:LEU:HD23 | 2:686:B:ARG:HA   | 1        | 0.4           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 4        | 0.4           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 4        | 0.4           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 4        | 0.4           |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 14       | 0.4           |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 14       | 0.4           |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 14       | 0.4           |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD21 | 12       | 0.4           |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD22 | 12       | 0.4           |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD23 | 12       | 0.4           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 9        | 0.4           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 9        | 0.4           |
| (1,788) | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 9        | 0.4           |
| (1,740) | 2:704:B:GLU:HG3  | 2:704:B:GLU:H    | 2        | 0.4           |
| (1,740) | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 10       | 0.4           |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 8        | 0.4           |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 8        | 0.4           |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 8        | 0.4           |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 12       | 0.4           |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 12       | 0.4           |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 12       | 0.4           |
| (1,589) | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 13       | 0.4           |
| (1,589) | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 13       | 0.4           |
| (1,589) | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 13       | 0.4           |
| (1,499) | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 5        | 0.4           |
| (1,463) | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 3        | 0.4           |
| (1,440) | 2:620:B:LEU:HD21 | 2:711:B:GLN:HG2  | 11       | 0.4           |
| (1,440) | 2:620:B:LEU:HD22 | 2:711:B:GLN:HG2  | 11       | 0.4           |
| (1,440) | 2:620:B:LEU:HD23 | 2:711:B:GLN:HG2  | 11       | 0.4           |
| (1,433) | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 2        | 0.4           |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE1  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE2  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE3  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE1  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE2  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE3  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE1  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE2  | 10       | 0.4           |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE3  | 10       | 0.4           |
| (1,317) | 2:712:B:ARG:HA   | 2:712:B:ARG:HD2  | 4        | 0.4           |
| (1,279) | 2:697:B:LEU:HD11 | 2:638:B:GLN:HG3  | 8        | 0.4           |
| (1,279) | 2:697:B:LEU:HD12 | 2:638:B:GLN:HG3  | 8        | 0.4           |
| (1,279) | 2:697:B:LEU:HD13 | 2:638:B:GLN:HG3  | 8        | 0.4           |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 11       | 0.4           |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 11       | 0.4           |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 11       | 0.4           |
| (1,175) | 2:640:B:LYS:HD3  | 2:637:B:ILE:HD11 | 3        | 0.4           |
| (1,175) | 2:640:B:LYS:HD3  | 2:637:B:ILE:HD12 | 3        | 0.4           |
| (1,175) | 2:640:B:LYS:HD3  | 2:637:B:ILE:HD13 | 3        | 0.4           |
| (1,174) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD11 | 1        | 0.4           |
| (1,174) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD12 | 1        | 0.4           |
| (1,174) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD13 | 1        | 0.4           |
| (1,172) | 2:665:B:ILE:HB   | 2:665:B:ILE:HD11 | 12       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,172)  | 2:665:B:ILE:HB   | 2:665:B:ILE:HD12 | 12       | 0.4           |
| (1,172)  | 2:665:B:ILE:HB   | 2:665:B:ILE:HD13 | 12       | 0.4           |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 15       | 0.4           |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 15       | 0.4           |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 15       | 0.4           |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 12       | 0.4           |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 12       | 0.4           |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 12       | 0.4           |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD11 | 17       | 0.4           |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD12 | 17       | 0.4           |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD13 | 17       | 0.4           |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 8        | 0.4           |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 8        | 0.4           |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 8        | 0.4           |
| (1,88)   | 2:647:B:GLU:HA   | 2:647:B:GLU:HG2  | 1        | 0.4           |
| (1,61)   | 2:632:B:ARG:HA   | 2:632:B:ARG:HG3  | 9        | 0.4           |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD21 | 8        | 0.4           |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD22 | 8        | 0.4           |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD23 | 8        | 0.4           |
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 18       | 0.4           |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 18       | 0.4           |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 18       | 0.4           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD21 | 2        | 0.39          |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD22 | 2        | 0.39          |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD23 | 2        | 0.39          |
| (1,2294) | 2:691:B:ILE:HG13 | 2:691:B:ILE:H    | 9        | 0.39          |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 9        | 0.39          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 8        | 0.39          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 12       | 0.39          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 15       | 0.39          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 8        | 0.39          |
| (1,1823) | 2:708:B:ARG:HG3  | 2:708:B:ARG:H    | 16       | 0.39          |
| (1,1570) | 2:647:B:GLU:HG2  | 2:647:B:GLU:HA   | 9        | 0.39          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 14       | 0.39          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 18       | 0.39          |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 5        | 0.39          |
| (1,1423) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HG3  | 4        | 0.39          |
| (1,1423) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HG3  | 4        | 0.39          |
| (1,1423) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HG3  | 4        | 0.39          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 11       | 0.39          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 20       | 0.39          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 20       | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 20       | 0.39          |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG21 | 5        | 0.39          |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG22 | 5        | 0.39          |
| (1,1116) | 2:624:B:LEU:HG   | 2:623:B:VAL:HG23 | 5        | 0.39          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 10       | 0.39          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 10       | 0.39          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 10       | 0.39          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 18       | 0.39          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 18       | 0.39          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 18       | 0.39          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 20       | 0.39          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 20       | 0.39          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 2        | 0.39          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 2        | 0.39          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 2        | 0.39          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 13       | 0.39          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 13       | 0.39          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 13       | 0.39          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 3        | 0.39          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 3        | 0.39          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 3        | 0.39          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 4        | 0.39          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 4        | 0.39          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 4        | 0.39          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 17       | 0.39          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 19       | 0.39          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 10       | 0.39          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 10       | 0.39          |
| (1,274)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 10       | 0.39          |
| (1,266)  | 2:631:B:ILE:HD11 | 2:634:B:LEU:HG   | 2        | 0.39          |
| (1,266)  | 2:631:B:ILE:HD12 | 2:634:B:LEU:HG   | 2        | 0.39          |
| (1,266)  | 2:631:B:ILE:HD13 | 2:634:B:LEU:HG   | 2        | 0.39          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE1  | 1        | 0.39          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE2  | 1        | 0.39          |
| (1,248)  | 2:703:B:LYS:HG2  | 2:702:B:MET:HE3  | 1        | 0.39          |
| (1,242)  | 2:692:B:ALA:HB1  | 2:688:B:ASN:HB2  | 5        | 0.39          |
| (1,242)  | 2:692:B:ALA:HB2  | 2:688:B:ASN:HB2  | 5        | 0.39          |
| (1,242)  | 2:692:B:ALA:HB3  | 2:688:B:ASN:HB2  | 5        | 0.39          |
| (1,210)  | 2:667:B:ARG:HB3  | 2:665:B:ILE:HG13 | 16       | 0.39          |
| (1,197)  | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 7        | 0.39          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG21 | 12       | 0.39          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG22 | 12       | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG23 | 12       | 0.39          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 1        | 0.39          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 1        | 0.39          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 1        | 0.39          |
| (1,136)  | 2:632:B:ARG:HB2  | 2:633:B:VAL:HG11 | 4        | 0.39          |
| (1,136)  | 2:632:B:ARG:HB2  | 2:633:B:VAL:HG12 | 4        | 0.39          |
| (1,136)  | 2:632:B:ARG:HB2  | 2:633:B:VAL:HG13 | 4        | 0.39          |
| (1,126)  | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG21 | 17       | 0.39          |
| (1,126)  | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG22 | 17       | 0.39          |
| (1,126)  | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG23 | 17       | 0.39          |
| (1,88)   | 2:647:B:GLU:HA   | 2:647:B:GLU:HG2  | 9        | 0.39          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD21 | 3        | 0.38          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD22 | 3        | 0.38          |
| (1,2662) | 2:703:B:LYS:HE3  | 1:211:A:LEU:HD23 | 3        | 0.38          |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD11 | 20       | 0.38          |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD12 | 20       | 0.38          |
| (1,2591) | 1:220:A:LEU:HA   | 1:220:A:LEU:HD13 | 20       | 0.38          |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 12       | 0.38          |
| (1,1873) | 2:608:B:GLU:HB2  | 2:608:B:GLU:H    | 14       | 0.38          |
| (1,1823) | 2:708:B:ARG:HG3  | 2:708:B:ARG:H    | 5        | 0.38          |
| (1,1817) | 2:709:B:GLU:HB3  | 2:710:B:ALA:H    | 10       | 0.38          |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG2  | 12       | 0.38          |
| (1,1626) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HA   | 12       | 0.38          |
| (1,1626) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HA   | 12       | 0.38          |
| (1,1626) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HA   | 12       | 0.38          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE3  | 11       | 0.38          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE3  | 11       | 0.38          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE3  | 11       | 0.38          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 4        | 0.38          |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 19       | 0.38          |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 14       | 0.38          |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 17       | 0.38          |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 18       | 0.38          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 6        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 6        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 6        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 7        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 7        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 7        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 8        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 8        | 0.38          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 8        | 0.38          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 10       | 0.38          |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 10       | 0.38          |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 10       | 0.38          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD21 | 2        | 0.38          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD22 | 2        | 0.38          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD23 | 2        | 0.38          |
| (1,746) | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 4        | 0.38          |
| (1,698) | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 1        | 0.38          |
| (1,698) | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 1        | 0.38          |
| (1,698) | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 1        | 0.38          |
| (1,672) | 2:677:B:LYS:HG3  | 2:678:B:ALA:H    | 9        | 0.38          |
| (1,672) | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 19       | 0.38          |
| (1,672) | 2:677:B:LYS:HD2  | 2:678:B:ALA:H    | 20       | 0.38          |
| (1,667) | 1:210:A:LEU:HD21 | 2:677:B:LYS:H    | 12       | 0.38          |
| (1,667) | 1:210:A:LEU:HD22 | 2:677:B:LYS:H    | 12       | 0.38          |
| (1,667) | 1:210:A:LEU:HD23 | 2:677:B:LYS:H    | 12       | 0.38          |
| (1,619) | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 17       | 0.38          |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 7        | 0.38          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 7        | 0.38          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 7        | 0.38          |
| (1,433) | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 15       | 0.38          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 15       | 0.38          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 15       | 0.38          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 15       | 0.38          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 15       | 0.38          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 15       | 0.38          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 15       | 0.38          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG21 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG22 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG23 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG21 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG22 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG23 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG21 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG22 | 7        | 0.38          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG23 | 7        | 0.38          |
| (1,179) | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG21 | 13       | 0.38          |
| (1,179) | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG22 | 13       | 0.38          |
| (1,179) | 2:700:B:LEU:HB2  | 2:631:B:ILE:HG23 | 13       | 0.38          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD11 | 6        | 0.38          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD12 | 6        | 0.38          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD13 | 6        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD11 | 18       | 0.38          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD12 | 18       | 0.38          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD13 | 18       | 0.38          |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG21 | 6        | 0.38          |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG22 | 6        | 0.38          |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG23 | 6        | 0.38          |
| (1,85)   | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 13       | 0.38          |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD3  | 10       | 0.38          |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD21 | 4        | 0.38          |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD22 | 4        | 0.38          |
| (1,55)   | 2:678:B:ALA:HA   | 2:670:B:LEU:HD23 | 4        | 0.38          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 7        | 0.38          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 7        | 0.38          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 7        | 0.38          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD2  | 5        | 0.38          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD2  | 5        | 0.38          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD2  | 5        | 0.38          |
| (1,12)   | 2:611:B:TYR:HD1  | 2:614:B:GLU:HA   | 8        | 0.38          |
| (1,12)   | 2:611:B:TYR:HD2  | 2:614:B:GLU:HA   | 8        | 0.38          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD21 | 16       | 0.37          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD22 | 16       | 0.37          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD23 | 16       | 0.37          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD21 | 17       | 0.37          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD22 | 17       | 0.37          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD23 | 17       | 0.37          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD21 | 17       | 0.37          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD22 | 17       | 0.37          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD23 | 17       | 0.37          |
| (1,2458) | 2:703:B:LYS:HG2  | 2:707:B:TRP:HE1  | 12       | 0.37          |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 14       | 0.37          |
| (1,2413) | 2:699:B:ARG:HG3  | 2:699:B:ARG:H    | 16       | 0.37          |
| (1,1713) | 2:686:B:ARG:HD3  | 2:683:B:ASP:HA   | 18       | 0.37          |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG2  | 13       | 0.37          |
| (1,1710) | 2:625:B:GLU:HA   | 2:625:B:GLU:HG3  | 8        | 0.37          |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE3  | 9        | 0.37          |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE3  | 9        | 0.37          |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE3  | 9        | 0.37          |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE2  | 15       | 0.37          |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE2  | 15       | 0.37          |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE2  | 15       | 0.37          |
| (1,1344) | 2:721:B:GLN:HB3  | 2:721:B:GLN:HG3  | 8        | 0.37          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD21 | 3        | 0.37          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,951) | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD22 | 3        | 0.37          |
| (1,951) | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD23 | 3        | 0.37          |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 7        | 0.37          |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 7        | 0.37          |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 7        | 0.37          |
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 3        | 0.37          |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 3        | 0.37          |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 3        | 0.37          |
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 17       | 0.37          |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 17       | 0.37          |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 17       | 0.37          |
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 20       | 0.37          |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 20       | 0.37          |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 20       | 0.37          |
| (1,756) | 2:620:B:LEU:HD21 | 2:707:B:TRP:HE1  | 1        | 0.37          |
| (1,756) | 2:620:B:LEU:HD22 | 2:707:B:TRP:HE1  | 1        | 0.37          |
| (1,756) | 2:620:B:LEU:HD23 | 2:707:B:TRP:HE1  | 1        | 0.37          |
| (1,698) | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 7        | 0.37          |
| (1,698) | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 7        | 0.37          |
| (1,698) | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 7        | 0.37          |
| (1,667) | 1:220:A:LEU:HD21 | 2:677:B:LYS:H    | 4        | 0.37          |
| (1,667) | 1:220:A:LEU:HD22 | 2:677:B:LYS:H    | 4        | 0.37          |
| (1,667) | 1:220:A:LEU:HD23 | 2:677:B:LYS:H    | 4        | 0.37          |
| (1,596) | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 6        | 0.37          |
| (1,596) | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 6        | 0.37          |
| (1,596) | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 6        | 0.37          |
| (1,535) | 2:716:B:LYS:HD2  | 2:720:B:GLU:H    | 12       | 0.37          |
| (1,514) | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 9        | 0.37          |
| (1,514) | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 9        | 0.37          |
| (1,514) | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 9        | 0.37          |
| (1,499) | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 4        | 0.37          |
| (1,260) | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG3  | 8        | 0.37          |
| (1,260) | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG3  | 8        | 0.37          |
| (1,260) | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG3  | 8        | 0.37          |
| (1,240) | 2:716:B:LYS:HG2  | 2:720:B:GLU:HG2  | 2        | 0.37          |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 6        | 0.37          |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 6        | 0.37          |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 6        | 0.37          |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD11 | 5        | 0.37          |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD12 | 5        | 0.37          |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD13 | 5        | 0.37          |
| (1,195) | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD11 | 5        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD12 | 5        | 0.37          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD13 | 5        | 0.37          |
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD11 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD12 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG21 | 2:658:B:LEU:HD13 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD11 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD12 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG22 | 2:658:B:LEU:HD13 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD11 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD12 | 2        | 0.37          |
| (1,150)  | 2:630:B:THR:HG23 | 2:658:B:LEU:HD13 | 2        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB1  | 2:693:B:VAL:HG21 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB1  | 2:693:B:VAL:HG22 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB1  | 2:693:B:VAL:HG23 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB2  | 2:693:B:VAL:HG21 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB2  | 2:693:B:VAL:HG22 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB2  | 2:693:B:VAL:HG23 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB3  | 2:693:B:VAL:HG21 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB3  | 2:693:B:VAL:HG22 | 7        | 0.37          |
| (1,134)  | 2:692:B:ALA:HB3  | 2:693:B:VAL:HG23 | 7        | 0.37          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 4        | 0.37          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 4        | 0.37          |
| (1,129)  | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 4        | 0.37          |
| (1,19)   | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 2        | 0.37          |
| (1,19)   | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 2        | 0.37          |
| (1,19)   | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 2        | 0.37          |
| (1,2710) | 1:213:A:ASP:HB2  | 1:214:A:GLU:H    | 2        | 0.36          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD21 | 2        | 0.36          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD22 | 2        | 0.36          |
| (1,2490) | 2:714:B:PHE:HD1  | 1:207:A:LEU:HD23 | 2        | 0.36          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD21 | 2        | 0.36          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD22 | 2        | 0.36          |
| (1,2490) | 2:714:B:PHE:HD2  | 1:207:A:LEU:HD23 | 2        | 0.36          |
| (1,2463) | 2:621:B:ASP:HA   | 2:711:B:GLN:HE22 | 15       | 0.36          |
| (1,2019) | 2:682:B:ILE:HG12 | 2:682:B:ILE:H    | 7        | 0.36          |
| (1,2019) | 2:682:B:ILE:HD11 | 2:682:B:ILE:H    | 16       | 0.36          |
| (1,2019) | 2:682:B:ILE:HD12 | 2:682:B:ILE:H    | 16       | 0.36          |
| (1,2019) | 2:682:B:ILE:HD13 | 2:682:B:ILE:H    | 16       | 0.36          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 1        | 0.36          |
| (1,1570) | 2:647:B:GLU:HG2  | 2:647:B:GLU:HA   | 4        | 0.36          |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 4        | 0.36          |
| (1,1423) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HG3  | 14       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1423) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HG3  | 14       | 0.36          |
| (1,1423) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HG3  | 14       | 0.36          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG3  | 2        | 0.36          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD11 | 11       | 0.36          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD12 | 11       | 0.36          |
| (1,1263) | 2:674:B:TYR:HE1  | 2:670:B:LEU:HD13 | 11       | 0.36          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD11 | 11       | 0.36          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD12 | 11       | 0.36          |
| (1,1263) | 2:674:B:TYR:HE2  | 2:670:B:LEU:HD13 | 11       | 0.36          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD21 | 12       | 0.36          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD22 | 12       | 0.36          |
| (1,951)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD23 | 12       | 0.36          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 17       | 0.36          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 17       | 0.36          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 17       | 0.36          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 13       | 0.36          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 13       | 0.36          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 13       | 0.36          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 19       | 0.36          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 19       | 0.36          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 19       | 0.36          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD21 | 17       | 0.36          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD22 | 17       | 0.36          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD23 | 17       | 0.36          |
| (1,740)  | 2:704:B:GLU:HG2  | 2:704:B:GLU:H    | 1        | 0.36          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 15       | 0.36          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 15       | 0.36          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 15       | 0.36          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 1        | 0.36          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 1        | 0.36          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 1        | 0.36          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 2        | 0.36          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 2        | 0.36          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 2        | 0.36          |
| (1,690)  | 2:685:B:LEU:HG   | 2:686:B:ARG:H    | 18       | 0.36          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 18       | 0.36          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 18       | 0.36          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 18       | 0.36          |
| (1,659)  | 2:670:B:LEU:HD21 | 2:674:B:TYR:H    | 17       | 0.36          |
| (1,659)  | 2:670:B:LEU:HD22 | 2:674:B:TYR:H    | 17       | 0.36          |
| (1,659)  | 2:670:B:LEU:HD23 | 2:674:B:TYR:H    | 17       | 0.36          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 11       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,464)  | 2:647:B:GLU:HA   | 2:649:B:GLN:HE21 | 16       | 0.36          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 8        | 0.36          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 8        | 0.36          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 8        | 0.36          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB1  | 2        | 0.36          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB2  | 2        | 0.36          |
| (1,251)  | 2:635:B:GLU:HB2  | 2:636:B:ALA:HB3  | 2        | 0.36          |
| (1,240)  | 2:716:B:LYS:HG2  | 2:720:B:GLU:HG2  | 1        | 0.36          |
| (1,235)  | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 19       | 0.36          |
| (1,235)  | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 19       | 0.36          |
| (1,235)  | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 19       | 0.36          |
| (1,226)  | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 1        | 0.36          |
| (1,197)  | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 17       | 0.36          |
| (1,155)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD11 | 18       | 0.36          |
| (1,155)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD12 | 18       | 0.36          |
| (1,155)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD13 | 18       | 0.36          |
| (1,133)  | 2:648:B:GLU:HG2  | 2:644:B:LEU:HD11 | 14       | 0.36          |
| (1,133)  | 2:648:B:GLU:HG2  | 2:644:B:LEU:HD12 | 14       | 0.36          |
| (1,133)  | 2:648:B:GLU:HG2  | 2:644:B:LEU:HD13 | 14       | 0.36          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 20       | 0.36          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 20       | 0.36          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 20       | 0.36          |
| (1,88)   | 2:647:B:GLU:HA   | 2:647:B:GLU:HG2  | 4        | 0.36          |
| (1,85)   | 2:625:B:GLU:HA   | 2:625:B:GLU:HG2  | 10       | 0.36          |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD2  | 2        | 0.36          |
| (1,2773) | 1:225:A:LYS:HG3  | 1:225:A:LYS:H    | 8        | 0.35          |
| (1,2710) | 1:213:A:ASP:HB2  | 1:214:A:GLU:H    | 14       | 0.35          |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE1  | 10       | 0.35          |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE2  | 10       | 0.35          |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE3  | 10       | 0.35          |
| (1,2294) | 2:691:B:ILE:HG13 | 2:691:B:ILE:H    | 3        | 0.35          |
| (1,2112) | 2:644:B:LEU:HD21 | 2:652:B:PHE:H    | 14       | 0.35          |
| (1,2112) | 2:644:B:LEU:HD22 | 2:652:B:PHE:H    | 14       | 0.35          |
| (1,2112) | 2:644:B:LEU:HD23 | 2:652:B:PHE:H    | 14       | 0.35          |
| (1,2112) | 2:644:B:LEU:HD21 | 2:652:B:PHE:H    | 17       | 0.35          |
| (1,2112) | 2:644:B:LEU:HD22 | 2:652:B:PHE:H    | 17       | 0.35          |
| (1,2112) | 2:644:B:LEU:HD23 | 2:652:B:PHE:H    | 17       | 0.35          |
| (1,2019) | 2:682:B:ILE:HG12 | 2:682:B:ILE:H    | 5        | 0.35          |
| (1,1818) | 2:708:B:ARG:HB2  | 2:709:B:GLU:H    | 5        | 0.35          |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG3  | 6        | 0.35          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB1  | 15       | 0.35          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB2  | 15       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB3  | 15       | 0.35          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB1  | 15       | 0.35          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB2  | 15       | 0.35          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB3  | 15       | 0.35          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB1  | 15       | 0.35          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB2  | 15       | 0.35          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB3  | 15       | 0.35          |
| (1,1626) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HA   | 13       | 0.35          |
| (1,1626) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HA   | 13       | 0.35          |
| (1,1626) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HA   | 13       | 0.35          |
| (1,1354) | 2:716:B:LYS:HD3  | 2:720:B:GLU:HG3  | 5        | 0.35          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 4        | 0.35          |
| (1,1289) | 2:689:B:PRO:HB3  | 2:653:B:ARG:HG3  | 2        | 0.35          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 2        | 0.35          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 2        | 0.35          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 2        | 0.35          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 18       | 0.35          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 18       | 0.35          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 18       | 0.35          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 5        | 0.35          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 5        | 0.35          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 5        | 0.35          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 9        | 0.35          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 9        | 0.35          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 9        | 0.35          |
| (1,754)  | 2:673:B:ILE:HG21 | 2:707:B:TRP:HE1  | 7        | 0.35          |
| (1,754)  | 2:673:B:ILE:HG22 | 2:707:B:TRP:HE1  | 7        | 0.35          |
| (1,754)  | 2:673:B:ILE:HG23 | 2:707:B:TRP:HE1  | 7        | 0.35          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 16       | 0.35          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 16       | 0.35          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 16       | 0.35          |
| (1,667)  | 1:210:A:LEU:HD21 | 2:677:B:LYS:H    | 5        | 0.35          |
| (1,667)  | 1:210:A:LEU:HD22 | 2:677:B:LYS:H    | 5        | 0.35          |
| (1,667)  | 1:210:A:LEU:HD23 | 2:677:B:LYS:H    | 5        | 0.35          |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 4        | 0.35          |
| (1,596)  | 2:637:B:ILE:HD11 | 2:636:B:ALA:H    | 3        | 0.35          |
| (1,596)  | 2:637:B:ILE:HD12 | 2:636:B:ALA:H    | 3        | 0.35          |
| (1,596)  | 2:637:B:ILE:HD13 | 2:636:B:ALA:H    | 3        | 0.35          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 14       | 0.35          |
| (1,463)  | 2:720:B:GLU:HA   | 2:721:B:GLN:HE22 | 20       | 0.35          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 8        | 0.35          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 8        | 0.35          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 8        | 0.35          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 8        | 0.35          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 8        | 0.35          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 8        | 0.35          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 8        | 0.35          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 8        | 0.35          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 8        | 0.35          |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE1  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE2  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE3  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE1  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE2  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE3  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE1  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE2  | 15       | 0.35          |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE3  | 15       | 0.35          |
| (1,409) | 2:620:B:LEU:HD11 | 2:711:B:GLN:HA   | 10       | 0.35          |
| (1,409) | 2:620:B:LEU:HD12 | 2:711:B:GLN:HA   | 10       | 0.35          |
| (1,409) | 2:620:B:LEU:HD13 | 2:711:B:GLN:HA   | 10       | 0.35          |
| (1,279) | 2:697:B:LEU:HD11 | 2:638:B:GLN:HG3  | 6        | 0.35          |
| (1,279) | 2:697:B:LEU:HD12 | 2:638:B:GLN:HG3  | 6        | 0.35          |
| (1,279) | 2:697:B:LEU:HD13 | 2:638:B:GLN:HG3  | 6        | 0.35          |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 7        | 0.35          |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 7        | 0.35          |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 7        | 0.35          |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 13       | 0.35          |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 13       | 0.35          |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 13       | 0.35          |
| (1,197) | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 2        | 0.35          |
| (1,197) | 2:644:B:LEU:HD21 | 2:649:B:GLN:HA   | 16       | 0.35          |
| (1,197) | 2:644:B:LEU:HD22 | 2:649:B:GLN:HA   | 16       | 0.35          |
| (1,197) | 2:644:B:LEU:HD23 | 2:649:B:GLN:HA   | 16       | 0.35          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD21 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD22 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD23 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD21 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD22 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD23 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD21 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD22 | 18       | 0.35          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD23 | 18       | 0.35          |
| (1,179) | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 2        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 2        | 0.35          |
| (1,179)  | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 2        | 0.35          |
| (1,175)  | 2:640:B:LYS:HD2  | 2:637:B:ILE:HD11 | 11       | 0.35          |
| (1,175)  | 2:640:B:LYS:HD2  | 2:637:B:ILE:HD12 | 11       | 0.35          |
| (1,175)  | 2:640:B:LYS:HD2  | 2:637:B:ILE:HD13 | 11       | 0.35          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 9        | 0.35          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 9        | 0.35          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 9        | 0.35          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 10       | 0.35          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 10       | 0.35          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 10       | 0.35          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 14       | 0.35          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 14       | 0.35          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 14       | 0.35          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD3  | 15       | 0.35          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD3  | 15       | 0.35          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD3  | 15       | 0.35          |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG21 | 13       | 0.34          |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG22 | 13       | 0.34          |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG23 | 13       | 0.34          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 16       | 0.34          |
| (1,2019) | 2:682:B:ILE:HD11 | 2:682:B:ILE:H    | 6        | 0.34          |
| (1,2019) | 2:682:B:ILE:HD12 | 2:682:B:ILE:H    | 6        | 0.34          |
| (1,2019) | 2:682:B:ILE:HD13 | 2:682:B:ILE:H    | 6        | 0.34          |
| (1,1710) | 2:625:B:GLU:HA   | 2:625:B:GLU:HG3  | 18       | 0.34          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 1        | 0.34          |
| (1,1548) | 2:672:B:ARG:HD3  | 2:672:B:ARG:HA   | 20       | 0.34          |
| (1,1354) | 2:716:B:LYS:HD3  | 2:720:B:GLU:HG3  | 13       | 0.34          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 19       | 0.34          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 19       | 0.34          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 19       | 0.34          |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG11 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG12 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG11 | 2:622:B:VAL:HG13 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG11 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG12 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG12 | 2:622:B:VAL:HG13 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG11 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG12 | 5        | 0.34          |
| (1,1223) | 2:623:B:VAL:HG13 | 2:622:B:VAL:HG13 | 5        | 0.34          |
| (1,920)  | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD21 | 15       | 0.34          |
| (1,920)  | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD22 | 15       | 0.34          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD23 | 15       | 0.34          |
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 1        | 0.34          |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 1        | 0.34          |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 1        | 0.34          |
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 4        | 0.34          |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 4        | 0.34          |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 4        | 0.34          |
| (1,821) | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 11       | 0.34          |
| (1,821) | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 11       | 0.34          |
| (1,821) | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 11       | 0.34          |
| (1,791) | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD21 | 18       | 0.34          |
| (1,791) | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD22 | 18       | 0.34          |
| (1,791) | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD23 | 18       | 0.34          |
| (1,763) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD11 | 16       | 0.34          |
| (1,763) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD12 | 16       | 0.34          |
| (1,763) | 2:675:B:ALA:HA   | 1:210:A:LEU:HD13 | 16       | 0.34          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD21 | 13       | 0.34          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD22 | 13       | 0.34          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD23 | 13       | 0.34          |
| (1,698) | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 5        | 0.34          |
| (1,698) | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 5        | 0.34          |
| (1,698) | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 5        | 0.34          |
| (1,688) | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 10       | 0.34          |
| (1,688) | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 10       | 0.34          |
| (1,688) | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 10       | 0.34          |
| (1,536) | 2:614:B:GLU:HB2  | 2:615:B:ASP:H    | 19       | 0.34          |
| (1,444) | 2:633:B:VAL:HB   | 2:658:B:LEU:HD21 | 12       | 0.34          |
| (1,444) | 2:633:B:VAL:HB   | 2:658:B:LEU:HD22 | 12       | 0.34          |
| (1,444) | 2:633:B:VAL:HB   | 2:658:B:LEU:HD23 | 12       | 0.34          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD11 | 18       | 0.34          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD12 | 18       | 0.34          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD13 | 18       | 0.34          |
| (1,278) | 2:685:B:LEU:HD11 | 2:696:B:VAL:HB   | 7        | 0.34          |
| (1,278) | 2:685:B:LEU:HD12 | 2:696:B:VAL:HB   | 7        | 0.34          |
| (1,278) | 2:685:B:LEU:HD13 | 2:696:B:VAL:HB   | 7        | 0.34          |
| (1,278) | 2:685:B:LEU:HD11 | 2:696:B:VAL:HB   | 14       | 0.34          |
| (1,278) | 2:685:B:LEU:HD12 | 2:696:B:VAL:HB   | 14       | 0.34          |
| (1,278) | 2:685:B:LEU:HD13 | 2:696:B:VAL:HB   | 14       | 0.34          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB1  | 6        | 0.34          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB2  | 6        | 0.34          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB3  | 6        | 0.34          |
| (1,242) | 2:692:B:ALA:HB1  | 2:688:B:ASN:HB2  | 2        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,242)  | 2:692:B:ALA:HB2  | 2:688:B:ASN:HB2  | 2        | 0.34          |
| (1,242)  | 2:692:B:ALA:HB3  | 2:688:B:ASN:HB2  | 2        | 0.34          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD11 | 14       | 0.34          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD12 | 14       | 0.34          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD13 | 14       | 0.34          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD11 | 14       | 0.34          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD12 | 14       | 0.34          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD13 | 14       | 0.34          |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD11 | 15       | 0.34          |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD12 | 15       | 0.34          |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD13 | 15       | 0.34          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 16       | 0.34          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 16       | 0.34          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 16       | 0.34          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 20       | 0.34          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 20       | 0.34          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 20       | 0.34          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD11 | 8        | 0.34          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD12 | 8        | 0.34          |
| (1,133)  | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD13 | 8        | 0.34          |
| (1,66)   | 2:636:B:ALA:HA   | 2:639:B:LYS:HD3  | 7        | 0.34          |
| (1,19)   | 2:682:B:ILE:HG21 | 2:681:B:ILE:HA   | 17       | 0.34          |
| (1,19)   | 2:682:B:ILE:HG22 | 2:681:B:ILE:HA   | 17       | 0.34          |
| (1,19)   | 2:682:B:ILE:HG23 | 2:681:B:ILE:HA   | 17       | 0.34          |
| (1,12)   | 2:611:B:TYR:HD1  | 2:616:B:GLU:HA   | 19       | 0.34          |
| (1,12)   | 2:611:B:TYR:HD2  | 2:616:B:GLU:HA   | 19       | 0.34          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD21 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD22 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD23 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD21 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD22 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD23 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD21 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD22 | 5        | 0.33          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD23 | 5        | 0.33          |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 1        | 0.33          |
| (1,2698) | 1:211:A:LEU:HB2  | 1:211:A:LEU:H    | 14       | 0.33          |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD11 | 17       | 0.33          |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD12 | 17       | 0.33          |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD13 | 17       | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 6        | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 6        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 6        | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 14       | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 14       | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 14       | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 18       | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 18       | 0.33          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 18       | 0.33          |
| (1,2197) | 2:677:B:LYS:HE2  | 2:677:B:LYS:H    | 2        | 0.33          |
| (1,2197) | 2:677:B:LYS:HE2  | 2:677:B:LYS:H    | 3        | 0.33          |
| (1,2046) | 2:643:B:ARG:HG2  | 2:643:B:ARG:H    | 15       | 0.33          |
| (1,1629) | 2:714:B:PHE:HD1  | 2:620:B:LEU:HD11 | 3        | 0.33          |
| (1,1629) | 2:714:B:PHE:HD1  | 2:620:B:LEU:HD12 | 3        | 0.33          |
| (1,1629) | 2:714:B:PHE:HD1  | 2:620:B:LEU:HD13 | 3        | 0.33          |
| (1,1629) | 2:714:B:PHE:HD2  | 2:620:B:LEU:HD11 | 3        | 0.33          |
| (1,1629) | 2:714:B:PHE:HD2  | 2:620:B:LEU:HD12 | 3        | 0.33          |
| (1,1629) | 2:714:B:PHE:HD2  | 2:620:B:LEU:HD13 | 3        | 0.33          |
| (1,1548) | 2:672:B:ARG:HD3  | 2:672:B:ARG:HA   | 19       | 0.33          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 5        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD21 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD22 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG11 | 2:620:B:LEU:HD23 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD21 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD22 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG12 | 2:620:B:LEU:HD23 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD21 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD22 | 3        | 0.33          |
| (1,1233) | 2:623:B:VAL:HG13 | 2:620:B:LEU:HD23 | 3        | 0.33          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 19       | 0.33          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 19       | 0.33          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 19       | 0.33          |
| (1,939)  | 2:639:B:LYS:HA   | 2:639:B:LYS:HG3  | 2        | 0.33          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD11 | 10       | 0.33          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD12 | 10       | 0.33          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD13 | 10       | 0.33          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 15       | 0.33          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 15       | 0.33          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 15       | 0.33          |
| (1,821)  | 2:644:B:LEU:HD11 | 2:644:B:LEU:HA   | 16       | 0.33          |
| (1,821)  | 2:644:B:LEU:HD12 | 2:644:B:LEU:HA   | 16       | 0.33          |
| (1,821)  | 2:644:B:LEU:HD13 | 2:644:B:LEU:HA   | 16       | 0.33          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD21 | 20       | 0.33          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD22 | 20       | 0.33          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,761) | 2:711:B:GLN:HA   | 1:207:A:LEU:HD23 | 20       | 0.33          |
| (1,754) | 2:673:B:ILE:HG21 | 2:707:B:TRP:HE1  | 8        | 0.33          |
| (1,754) | 2:673:B:ILE:HG22 | 2:707:B:TRP:HE1  | 8        | 0.33          |
| (1,754) | 2:673:B:ILE:HG23 | 2:707:B:TRP:HE1  | 8        | 0.33          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 12       | 0.33          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 12       | 0.33          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 12       | 0.33          |
| (1,672) | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 4        | 0.33          |
| (1,672) | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 13       | 0.33          |
| (1,672) | 2:677:B:LYS:HD3  | 2:678:B:ALA:H    | 14       | 0.33          |
| (1,619) | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 5        | 0.33          |
| (1,468) | 2:726:B:TYR:HB2  | 2:726:B:TYR:H    | 4        | 0.33          |
| (1,463) | 2:720:B:GLU:HA   | 2:721:B:GLN:HE22 | 4        | 0.33          |
| (1,433) | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 6        | 0.33          |
| (1,433) | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 9        | 0.33          |
| (1,416) | 1:222:A:THR:HA   | 2:695:B:ILE:HD11 | 5        | 0.33          |
| (1,416) | 1:222:A:THR:HA   | 2:695:B:ILE:HD12 | 5        | 0.33          |
| (1,416) | 1:222:A:THR:HA   | 2:695:B:ILE:HD13 | 5        | 0.33          |
| (1,289) | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB2  | 14       | 0.33          |
| (1,289) | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB2  | 14       | 0.33          |
| (1,289) | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB2  | 14       | 0.33          |
| (1,267) | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD2  | 14       | 0.33          |
| (1,267) | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD2  | 14       | 0.33          |
| (1,267) | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD2  | 14       | 0.33          |
| (1,256) | 2:658:B:LEU:HD21 | 2:630:B:THR:HG21 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD21 | 2:630:B:THR:HG22 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD21 | 2:630:B:THR:HG23 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD22 | 2:630:B:THR:HG21 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD22 | 2:630:B:THR:HG22 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD22 | 2:630:B:THR:HG23 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD23 | 2:630:B:THR:HG21 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD23 | 2:630:B:THR:HG22 | 12       | 0.33          |
| (1,256) | 2:658:B:LEU:HD23 | 2:630:B:THR:HG23 | 12       | 0.33          |
| (1,214) | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 2        | 0.33          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 12       | 0.33          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 12       | 0.33          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 12       | 0.33          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 12       | 0.33          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 12       | 0.33          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 12       | 0.33          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 12       | 0.33          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 12       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 12       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 13       | 0.33          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 13       | 0.33          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG21 | 10       | 0.33          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG22 | 10       | 0.33          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG23 | 10       | 0.33          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 3        | 0.33          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 3        | 0.33          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 3        | 0.33          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 5        | 0.33          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 5        | 0.33          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 5        | 0.33          |
| (1,16)   | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD3  | 6        | 0.33          |
| (1,16)   | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD3  | 6        | 0.33          |
| (1,16)   | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD3  | 6        | 0.33          |
| (1,15)   | 2:664:B:VAL:HG21 | 2:667:B:ARG:HD3  | 16       | 0.33          |
| (1,15)   | 2:664:B:VAL:HG22 | 2:667:B:ARG:HD3  | 16       | 0.33          |
| (1,15)   | 2:664:B:VAL:HG23 | 2:667:B:ARG:HD3  | 16       | 0.33          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG11 | 2        | 0.32          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG12 | 2        | 0.32          |
| (2,9)    | 2:662:B:SER:HB2  | 2:633:B:VAL:HG13 | 2        | 0.32          |
| (1,2749) | 1:221:A:ARG:HG3  | 1:221:A:ARG:H    | 6        | 0.32          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 4        | 0.32          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 4        | 0.32          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 4        | 0.32          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 17       | 0.32          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 17       | 0.32          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 17       | 0.32          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 3        | 0.32          |
| (1,1873) | 2:608:B:GLU:HB2  | 2:608:B:GLU:H    | 11       | 0.32          |
| (1,1711) | 2:663:B:GLU:HA   | 2:663:B:GLU:HG2  | 3        | 0.32          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 8        | 0.32          |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 15       | 0.32          |
| (1,1354) | 2:716:B:LYS:HD3  | 2:720:B:GLU:HG3  | 7        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD11 | 2        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD12 | 2        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD13 | 2        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD11 | 2        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD12 | 2        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD13 | 2        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD11 | 2        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD12 | 2        | 0.32          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD13 | 2        | 0.32          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 7        | 0.32          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 7        | 0.32          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 7        | 0.32          |
| (1,1026) | 2:706:B:GLU:HA   | 2:709:B:GLU:HG3  | 9        | 0.32          |
| (1,1019) | 2:698:B:LYS:HA   | 2:698:B:LYS:HB3  | 1        | 0.32          |
| (1,684)  | 2:716:B:LYS:HD3  | 2:717:B:VAL:H    | 10       | 0.32          |
| (1,637)  | 2:654:B:LEU:HD21 | 2:658:B:LEU:H    | 2        | 0.32          |
| (1,637)  | 2:654:B:LEU:HD22 | 2:658:B:LEU:H    | 2        | 0.32          |
| (1,637)  | 2:654:B:LEU:HD23 | 2:658:B:LEU:H    | 2        | 0.32          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 10       | 0.32          |
| (1,463)  | 2:720:B:GLU:HA   | 2:721:B:GLN:HE22 | 16       | 0.32          |
| (1,384)  | 2:697:B:LEU:HD11 | 2:694:B:PRO:HA   | 17       | 0.32          |
| (1,384)  | 2:697:B:LEU:HD12 | 2:694:B:PRO:HA   | 17       | 0.32          |
| (1,384)  | 2:697:B:LEU:HD13 | 2:694:B:PRO:HA   | 17       | 0.32          |
| (1,371)  | 2:668:B:LYS:HB3  | 2:668:B:LYS:HA   | 3        | 0.32          |
| (1,371)  | 2:668:B:LYS:HB3  | 2:668:B:LYS:HA   | 10       | 0.32          |
| (1,371)  | 2:668:B:LYS:HB3  | 2:668:B:LYS:HA   | 19       | 0.32          |
| (1,316)  | 2:716:B:LYS:HA   | 2:719:B:ARG:HD3  | 15       | 0.32          |
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 13       | 0.32          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 13       | 0.32          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 13       | 0.32          |
| (1,278)  | 2:685:B:LEU:HD11 | 2:696:B:VAL:HB   | 20       | 0.32          |
| (1,278)  | 2:685:B:LEU:HD12 | 2:696:B:VAL:HB   | 20       | 0.32          |
| (1,278)  | 2:685:B:LEU:HD13 | 2:696:B:VAL:HB   | 20       | 0.32          |
| (1,197)  | 2:641:B:LEU:HD11 | 2:649:B:GLN:HA   | 14       | 0.32          |
| (1,197)  | 2:641:B:LEU:HD12 | 2:649:B:GLN:HA   | 14       | 0.32          |
| (1,197)  | 2:641:B:LEU:HD13 | 2:649:B:GLN:HA   | 14       | 0.32          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD11 | 14       | 0.32          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD12 | 14       | 0.32          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD13 | 14       | 0.32          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 20       | 0.32          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 20       | 0.32          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 20       | 0.32          |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG21 | 15       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG22 | 15       | 0.32          |
| (1,126)  | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG23 | 15       | 0.32          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 4        | 0.32          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 4        | 0.32          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 4        | 0.32          |
| (1,85)   | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 4        | 0.32          |
| (1,74)   | 2:613:B:CYS:HB3  | 2:612:B:ARG:HB2  | 7        | 0.32          |
| (1,61)   | 2:632:B:ARG:HA   | 2:632:B:ARG:HG3  | 8        | 0.32          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD21 | 9        | 0.32          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD22 | 9        | 0.32          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD23 | 9        | 0.32          |
| (1,17)   | 2:624:B:LEU:HD21 | 2:708:B:ARG:HD3  | 12       | 0.32          |
| (1,17)   | 2:624:B:LEU:HD22 | 2:708:B:ARG:HD3  | 12       | 0.32          |
| (1,17)   | 2:624:B:LEU:HD23 | 2:708:B:ARG:HD3  | 12       | 0.32          |
| (1,13)   | 2:682:B:ILE:HG21 | 2:686:B:ARG:HD3  | 6        | 0.32          |
| (1,13)   | 2:682:B:ILE:HG22 | 2:686:B:ARG:HD3  | 6        | 0.32          |
| (1,13)   | 2:682:B:ILE:HG23 | 2:686:B:ARG:HD3  | 6        | 0.32          |
| (1,2749) | 1:221:A:ARG:HG3  | 1:221:A:ARG:H    | 15       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD11 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD12 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG21 | 1:220:A:LEU:HD13 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD11 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD12 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG22 | 1:220:A:LEU:HD13 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD11 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD12 | 16       | 0.31          |
| (1,2603) | 2:681:B:ILE:HG23 | 1:220:A:LEU:HD13 | 16       | 0.31          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE1  | 8        | 0.31          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE2  | 8        | 0.31          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE3  | 8        | 0.31          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 20       | 0.31          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 20       | 0.31          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 20       | 0.31          |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 13       | 0.31          |
| (1,1838) | 2:615:B:ASP:HB2  | 2:616:B:GLU:H    | 12       | 0.31          |
| (1,1605) | 2:643:B:ARG:HB3  | 2:643:B:ARG:HD3  | 5        | 0.31          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 9        | 0.31          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 12       | 0.31          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 9        | 0.31          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 9        | 0.31          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 9        | 0.31          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 9        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 9        | 0.31          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 9        | 0.31          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 9        | 0.31          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 9        | 0.31          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 9        | 0.31          |
| (1,1141) | 2:620:B:LEU:HB3  | 2:623:B:VAL:HG11 | 5        | 0.31          |
| (1,1141) | 2:620:B:LEU:HB3  | 2:623:B:VAL:HG12 | 5        | 0.31          |
| (1,1141) | 2:620:B:LEU:HB3  | 2:623:B:VAL:HG13 | 5        | 0.31          |
| (1,1138) | 2:656:B:ASN:HB2  | 2:657:B:THR:HG21 | 4        | 0.31          |
| (1,1138) | 2:656:B:ASN:HB2  | 2:657:B:THR:HG22 | 4        | 0.31          |
| (1,1138) | 2:656:B:ASN:HB2  | 2:657:B:THR:HG23 | 4        | 0.31          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 12       | 0.31          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 12       | 0.31          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 12       | 0.31          |
| (1,997)  | 2:668:B:LYS:HA   | 2:668:B:LYS:HD2  | 5        | 0.31          |
| (1,761)  | 2:620:B:LEU:HA   | 1:207:A:LEU:HD21 | 17       | 0.31          |
| (1,761)  | 2:620:B:LEU:HA   | 1:207:A:LEU:HD22 | 17       | 0.31          |
| (1,761)  | 2:620:B:LEU:HA   | 1:207:A:LEU:HD23 | 17       | 0.31          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD21 | 9        | 0.31          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD22 | 9        | 0.31          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD23 | 9        | 0.31          |
| (1,616)  | 2:643:B:ARG:HG3  | 2:643:B:ARG:H    | 13       | 0.31          |
| (1,521)  | 2:675:B:ALA:HB1  | 2:677:B:LYS:H    | 4        | 0.31          |
| (1,521)  | 2:675:B:ALA:HB2  | 2:677:B:LYS:H    | 4        | 0.31          |
| (1,521)  | 2:675:B:ALA:HB3  | 2:677:B:LYS:H    | 4        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE1  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE2  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG21 | 2:702:B:MET:HE3  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE1  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE2  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG22 | 2:702:B:MET:HE3  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE1  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE2  | 8        | 0.31          |
| (1,415)  | 2:673:B:ILE:HG23 | 2:702:B:MET:HE3  | 8        | 0.31          |
| (1,384)  | 2:697:B:LEU:HD11 | 2:694:B:PRO:HA   | 1        | 0.31          |
| (1,384)  | 2:697:B:LEU:HD12 | 2:694:B:PRO:HA   | 1        | 0.31          |
| (1,384)  | 2:697:B:LEU:HD13 | 2:694:B:PRO:HA   | 1        | 0.31          |
| (1,384)  | 2:697:B:LEU:HD11 | 2:694:B:PRO:HA   | 20       | 0.31          |
| (1,384)  | 2:697:B:LEU:HD12 | 2:694:B:PRO:HA   | 20       | 0.31          |
| (1,384)  | 2:697:B:LEU:HD13 | 2:694:B:PRO:HA   | 20       | 0.31          |
| (1,345)  | 2:616:B:GLU:HB2  | 2:616:B:GLU:HA   | 9        | 0.31          |
| (1,269)  | 2:633:B:VAL:HG21 | 2:632:B:ARG:HB3  | 4        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,269)  | 2:633:B:VAL:HG22 | 2:632:B:ARG:HB3  | 4        | 0.31          |
| (1,269)  | 2:633:B:VAL:HG23 | 2:632:B:ARG:HB3  | 4        | 0.31          |
| (1,235)  | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 2        | 0.31          |
| (1,235)  | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 2        | 0.31          |
| (1,235)  | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 2        | 0.31          |
| (1,214)  | 2:670:B:LEU:HB2  | 2:634:B:LEU:HG   | 18       | 0.31          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 19       | 0.31          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 19       | 0.31          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 19       | 0.31          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 19       | 0.31          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 19       | 0.31          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 19       | 0.31          |
| (1,183)  | 2:667:B:ARG:HG3  | 2:682:B:ILE:HG21 | 17       | 0.31          |
| (1,183)  | 2:667:B:ARG:HG3  | 2:682:B:ILE:HG22 | 17       | 0.31          |
| (1,183)  | 2:667:B:ARG:HG3  | 2:682:B:ILE:HG23 | 17       | 0.31          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 18       | 0.31          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 18       | 0.31          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 18       | 0.31          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 1        | 0.31          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 1        | 0.31          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 1        | 0.31          |
| (1,85)   | 2:625:B:GLU:HA   | 2:625:B:GLU:HG2  | 15       | 0.31          |
| (1,85)   | 2:625:B:GLU:HA   | 2:625:B:GLU:HG2  | 19       | 0.31          |
| (1,14)   | 2:658:B:LEU:HD21 | 2:686:B:ARG:HD2  | 4        | 0.31          |
| (1,14)   | 2:658:B:LEU:HD22 | 2:686:B:ARG:HD2  | 4        | 0.31          |
| (1,14)   | 2:658:B:LEU:HD23 | 2:686:B:ARG:HD2  | 4        | 0.31          |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD21 | 1        | 0.3           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD22 | 1        | 0.3           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD23 | 1        | 0.3           |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 1        | 0.3           |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 1        | 0.3           |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 1        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD21 | 1:205:A:ALA:HB1  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD21 | 1:205:A:ALA:HB2  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD21 | 1:205:A:ALA:HB3  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD22 | 1:205:A:ALA:HB1  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD22 | 1:205:A:ALA:HB2  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD22 | 1:205:A:ALA:HB3  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD23 | 1:205:A:ALA:HB1  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD23 | 1:205:A:ALA:HB2  | 3        | 0.3           |
| (1,2467) | 1:207:A:LEU:HD23 | 1:205:A:ALA:HB3  | 3        | 0.3           |
| (1,2125) | 2:613:B:CYS:HB2  | 2:615:B:ASP:H    | 10       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 3        | 0.3           |
| (1,2019) | 2:682:B:ILE:HG12 | 2:682:B:ILE:H    | 9        | 0.3           |
| (1,1852) | 2:701:B:LYS:HD3  | 2:700:B:LEU:H    | 2        | 0.3           |
| (1,1407) | 2:644:B:LEU:HD21 | 2:648:B:GLU:HB3  | 11       | 0.3           |
| (1,1407) | 2:644:B:LEU:HD22 | 2:648:B:GLU:HB3  | 11       | 0.3           |
| (1,1407) | 2:644:B:LEU:HD23 | 2:648:B:GLU:HB3  | 11       | 0.3           |
| (1,1354) | 2:716:B:LYS:HD3  | 2:720:B:GLU:HG3  | 18       | 0.3           |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 8        | 0.3           |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 2        | 0.3           |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 2        | 0.3           |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 2        | 0.3           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 16       | 0.3           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 16       | 0.3           |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 16       | 0.3           |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 11       | 0.3           |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 11       | 0.3           |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 11       | 0.3           |
| (1,1097) | 2:703:B:LYS:HE3  | 2:673:B:ILE:HG21 | 20       | 0.3           |
| (1,1097) | 2:703:B:LYS:HE3  | 2:673:B:ILE:HG22 | 20       | 0.3           |
| (1,1097) | 2:703:B:LYS:HE3  | 2:673:B:ILE:HG23 | 20       | 0.3           |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD11 | 8        | 0.3           |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD12 | 8        | 0.3           |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD13 | 8        | 0.3           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 16       | 0.3           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 16       | 0.3           |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 16       | 0.3           |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 3        | 0.3           |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 10       | 0.3           |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 16       | 0.3           |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 4        | 0.3           |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 4        | 0.3           |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 4        | 0.3           |
| (1,672)  | 2:677:B:LYS:HG3  | 2:678:B:ALA:H    | 2        | 0.3           |
| (1,667)  | 1:220:A:LEU:HD21 | 2:677:B:LYS:H    | 7        | 0.3           |
| (1,667)  | 1:220:A:LEU:HD22 | 2:677:B:LYS:H    | 7        | 0.3           |
| (1,667)  | 1:220:A:LEU:HD23 | 2:677:B:LYS:H    | 7        | 0.3           |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 8        | 0.3           |
| (1,536)  | 2:614:B:GLU:HB2  | 2:615:B:ASP:H    | 7        | 0.3           |
| (1,371)  | 2:647:B:GLU:HB2  | 2:647:B:GLU:HA   | 14       | 0.3           |
| (1,341)  | 2:635:B:GLU:HB3  | 2:635:B:GLU:HA   | 7        | 0.3           |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 7        | 0.3           |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 7        | 0.3           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 7        | 0.3           |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 7        | 0.3           |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 7        | 0.3           |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 7        | 0.3           |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 7        | 0.3           |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 7        | 0.3           |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 7        | 0.3           |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 14       | 0.3           |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 14       | 0.3           |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 14       | 0.3           |
| (1,238) | 2:716:B:LYS:HG3  | 2:720:B:GLU:HG3  | 6        | 0.3           |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD11 | 11       | 0.3           |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD12 | 11       | 0.3           |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD13 | 11       | 0.3           |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD11 | 17       | 0.3           |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD12 | 17       | 0.3           |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD13 | 17       | 0.3           |
| (1,195) | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD11 | 17       | 0.3           |
| (1,195) | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD12 | 17       | 0.3           |
| (1,195) | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD13 | 17       | 0.3           |
| (1,190) | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG11 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG12 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG13 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG11 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG12 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG13 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG11 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG12 | 6        | 0.3           |
| (1,190) | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG13 | 6        | 0.3           |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 8        | 0.3           |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 19       | 0.3           |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 19       | 0.3           |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 19       | 0.3           |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 19       | 0.3           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 19       | 0.3           |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 19       | 0.3           |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 19       | 0.3           |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 19       | 0.3           |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 19       | 0.3           |
| (1,187) | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG11 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG12 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD21 | 2:623:B:VAL:HG13 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG11 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG12 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD22 | 2:623:B:VAL:HG13 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG11 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG12 | 16       | 0.3           |
| (1,187) | 2:620:B:LEU:HD23 | 2:623:B:VAL:HG13 | 16       | 0.3           |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD21 | 8        | 0.3           |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD22 | 8        | 0.3           |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD23 | 8        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 2        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 2        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 2        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 3        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 3        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 3        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 4        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 4        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 4        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 6        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 6        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 6        | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 10       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 10       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 10       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 14       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 14       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 14       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 19       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 19       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 19       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 20       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 20       | 0.3           |
| (1,147) | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 20       | 0.3           |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 20       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 20       | 0.3           |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 20       | 0.3           |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 17       | 0.3           |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 17       | 0.3           |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 17       | 0.3           |
| (1,15)   | 2:682:B:ILE:HD11 | 2:667:B:ARG:HD3  | 4        | 0.3           |
| (1,15)   | 2:682:B:ILE:HD12 | 2:667:B:ARG:HD3  | 4        | 0.3           |
| (1,15)   | 2:682:B:ILE:HD13 | 2:667:B:ARG:HD3  | 4        | 0.3           |
| (1,12)   | 2:718:B:TRP:HZ3  | 2:723:B:GLU:HA   | 20       | 0.3           |
| (1,2509) | 1:211:A:LEU:HD21 | 1:211:A:LEU:HA   | 13       | 0.29          |
| (1,2509) | 1:211:A:LEU:HD22 | 1:211:A:LEU:HA   | 13       | 0.29          |
| (1,2509) | 1:211:A:LEU:HD23 | 1:211:A:LEU:HA   | 13       | 0.29          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 7        | 0.29          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 7        | 0.29          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 7        | 0.29          |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 18       | 0.29          |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 18       | 0.29          |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 18       | 0.29          |
| (1,2125) | 2:613:B:CYS:HB2  | 2:615:B:ASP:H    | 1        | 0.29          |
| (1,2125) | 2:613:B:CYS:HB3  | 2:615:B:ASP:H    | 16       | 0.29          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 13       | 0.29          |
| (1,1944) | 2:623:B:VAL:HG11 | 2:623:B:VAL:H    | 5        | 0.29          |
| (1,1944) | 2:623:B:VAL:HG12 | 2:623:B:VAL:H    | 5        | 0.29          |
| (1,1944) | 2:623:B:VAL:HG13 | 2:623:B:VAL:H    | 5        | 0.29          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 10       | 0.29          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 19       | 0.29          |
| (1,1783) | 2:727:B:LEU:HB2  | 2:727:B:LEU:H    | 10       | 0.29          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 5        | 0.29          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 5        | 0.29          |
| (1,1672) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HE3  | 8        | 0.29          |
| (1,1672) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HE3  | 8        | 0.29          |
| (1,1672) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HE3  | 8        | 0.29          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE3  | 20       | 0.29          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE3  | 20       | 0.29          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE3  | 20       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1561) | 2:716:B:LYS:HD3  | 2:716:B:LYS:HA   | 10       | 0.29          |
| (1,1475) | 2:667:B:ARG:HA   | 2:667:B:ARG:HD2  | 7        | 0.29          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 4        | 0.29          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 13       | 0.29          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 16       | 0.29          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 15       | 0.29          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD21 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD22 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG21 | 2:620:B:LEU:HD23 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD21 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD22 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG22 | 2:620:B:LEU:HD23 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD21 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD22 | 8        | 0.29          |
| (1,1231) | 2:623:B:VAL:HG23 | 2:620:B:LEU:HD23 | 8        | 0.29          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 17       | 0.29          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 17       | 0.29          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 17       | 0.29          |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD21 | 14       | 0.29          |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD22 | 14       | 0.29          |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD23 | 14       | 0.29          |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD21 | 16       | 0.29          |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD22 | 16       | 0.29          |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD23 | 16       | 0.29          |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD21 | 19       | 0.29          |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD22 | 19       | 0.29          |
| (1,791)  | 2:681:B:ILE:HA   | 1:223:A:LEU:HD23 | 19       | 0.29          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 1        | 0.29          |
| (1,668)  | 2:716:B:LYS:HA   | 2:718:B:TRP:H    | 20       | 0.29          |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 10       | 0.29          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 10       | 0.29          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 11       | 0.29          |
| (1,464)  | 2:647:B:GLU:HA   | 2:649:B:GLN:HE21 | 20       | 0.29          |
| (1,432)  | 2:664:B:VAL:HB   | 2:668:B:LYS:HE3  | 13       | 0.29          |
| (1,403)  | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD3  | 5        | 0.29          |
| (1,388)  | 2:648:B:GLU:HB3  | 2:651:B:LYS:HE2  | 11       | 0.29          |
| (1,316)  | 2:716:B:LYS:HA   | 2:719:B:ARG:HD2  | 4        | 0.29          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 15       | 0.29          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 15       | 0.29          |
| (1,274)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 15       | 0.29          |
| (1,226)  | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 16       | 0.29          |
| (1,220)  | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 13       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,220)  | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 16       | 0.29          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 4        | 0.29          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 4        | 0.29          |
| (1,195)  | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 4        | 0.29          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 4        | 0.29          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 4        | 0.29          |
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 4        | 0.29          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 17       | 0.29          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 17       | 0.29          |
| (1,159)  | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 17       | 0.29          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 8        | 0.29          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 8        | 0.29          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 8        | 0.29          |
| (1,147)  | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD21 | 7        | 0.29          |
| (1,147)  | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD22 | 7        | 0.29          |
| (1,147)  | 2:634:B:LEU:HB3  | 2:634:B:LEU:HD23 | 7        | 0.29          |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD3  | 5        | 0.29          |
| (1,17)   | 2:624:B:LEU:HD21 | 2:708:B:ARG:HD3  | 19       | 0.29          |
| (1,17)   | 2:624:B:LEU:HD22 | 2:708:B:ARG:HD3  | 19       | 0.29          |
| (1,17)   | 2:624:B:LEU:HD23 | 2:708:B:ARG:HD3  | 19       | 0.29          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD21 | 5        | 0.28          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD22 | 5        | 0.28          |
| (1,2503) | 1:210:A:LEU:HA   | 1:210:A:LEU:HD23 | 5        | 0.28          |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 9        | 0.28          |
| (1,2302) | 2:693:B:VAL:HG21 | 2:693:B:VAL:H    | 7        | 0.28          |
| (1,2302) | 2:693:B:VAL:HG22 | 2:693:B:VAL:H    | 7        | 0.28          |
| (1,2302) | 2:693:B:VAL:HG23 | 2:693:B:VAL:H    | 7        | 0.28          |
| (1,2239) | 2:687:B:LYS:HE2  | 2:684:B:GLY:H    | 4        | 0.28          |
| (1,2079) | 2:649:B:GLN:HG3  | 2:649:B:GLN:H    | 14       | 0.28          |
| (1,1911) | 2:724:B:LYS:HB2  | 2:724:B:LYS:H    | 12       | 0.28          |
| (1,1783) | 2:727:B:LEU:HB2  | 2:727:B:LEU:H    | 1        | 0.28          |
| (1,1750) | 2:667:B:ARG:HG3  | 2:671:B:GLN:HE22 | 12       | 0.28          |
| (1,1423) | 2:697:B:LEU:HD11 | 2:635:B:GLU:HG3  | 12       | 0.28          |
| (1,1423) | 2:697:B:LEU:HD12 | 2:635:B:GLU:HG3  | 12       | 0.28          |
| (1,1423) | 2:697:B:LEU:HD13 | 2:635:B:GLU:HG3  | 12       | 0.28          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD2  | 5        | 0.28          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD2  | 5        | 0.28          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD2  | 5        | 0.28          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG3  | 15       | 0.28          |
| (1,939)  | 2:639:B:LYS:HA   | 2:639:B:LYS:HG3  | 1        | 0.28          |
| (1,937)  | 2:669:B:ALA:HA   | 2:668:B:LYS:HG3  | 12       | 0.28          |
| (1,921)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD11 | 4        | 0.28          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,921) | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD12 | 4        | 0.28          |
| (1,921) | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD13 | 4        | 0.28          |
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD21 | 20       | 0.28          |
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD22 | 20       | 0.28          |
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD23 | 20       | 0.28          |
| (1,899) | 2:620:B:LEU:HA   | 2:623:B:VAL:HG11 | 16       | 0.28          |
| (1,899) | 2:620:B:LEU:HA   | 2:623:B:VAL:HG12 | 16       | 0.28          |
| (1,899) | 2:620:B:LEU:HA   | 2:623:B:VAL:HG13 | 16       | 0.28          |
| (1,791) | 2:681:B:ILE:HA   | 1:223:A:LEU:HD21 | 1        | 0.28          |
| (1,791) | 2:681:B:ILE:HA   | 1:223:A:LEU:HD22 | 1        | 0.28          |
| (1,791) | 2:681:B:ILE:HA   | 1:223:A:LEU:HD23 | 1        | 0.28          |
| (1,746) | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 8        | 0.28          |
| (1,746) | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 14       | 0.28          |
| (1,697) | 2:687:B:LYS:HD3  | 2:688:B:ASN:H    | 18       | 0.28          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 6        | 0.28          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 6        | 0.28          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 6        | 0.28          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 7        | 0.28          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 7        | 0.28          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 7        | 0.28          |
| (1,614) | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 17       | 0.28          |
| (1,613) | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 6        | 0.28          |
| (1,609) | 2:641:B:LEU:HB3  | 2:641:B:LEU:H    | 6        | 0.28          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 1        | 0.28          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 1        | 0.28          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD3  | 7        | 0.28          |
| (1,394) | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE3  | 20       | 0.28          |
| (1,394) | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE3  | 20       | 0.28          |
| (1,394) | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE3  | 20       | 0.28          |
| (1,364) | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 2        | 0.28          |
| (1,364) | 2:639:B:LYS:HB2  | 2:639:B:LYS:HA   | 10       | 0.28          |
| (1,295) | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB1  | 12       | 0.28          |
| (1,295) | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB2  | 12       | 0.28          |
| (1,295) | 2:624:B:LEU:HD21 | 2:710:B:ALA:HB3  | 12       | 0.28          |
| (1,295) | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB1  | 12       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB2  | 12       | 0.28          |
| (1,295)  | 2:624:B:LEU:HD22 | 2:710:B:ALA:HB3  | 12       | 0.28          |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB1  | 12       | 0.28          |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB2  | 12       | 0.28          |
| (1,295)  | 2:624:B:LEU:HD23 | 2:710:B:ALA:HB3  | 12       | 0.28          |
| (1,242)  | 2:673:B:ILE:HG21 | 2:674:B:TYR:HB2  | 8        | 0.28          |
| (1,242)  | 2:673:B:ILE:HG22 | 2:674:B:TYR:HB2  | 8        | 0.28          |
| (1,242)  | 2:673:B:ILE:HG23 | 2:674:B:TYR:HB2  | 8        | 0.28          |
| (1,220)  | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB2  | 8        | 0.28          |
| (1,220)  | 2:647:B:GLU:HG3  | 2:647:B:GLU:HB3  | 15       | 0.28          |
| (1,197)  | 2:631:B:ILE:HG12 | 2:704:B:GLU:HA   | 20       | 0.28          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 3        | 0.28          |
| (1,188)  | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 3        | 0.28          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 10       | 0.28          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 10       | 0.28          |
| (1,158)  | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 10       | 0.28          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 11       | 0.28          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 11       | 0.28          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 11       | 0.28          |
| (1,96)   | 2:629:B:ALA:HA   | 2:665:B:ILE:HD11 | 12       | 0.28          |
| (1,96)   | 2:629:B:ALA:HA   | 2:665:B:ILE:HD12 | 12       | 0.28          |
| (1,96)   | 2:629:B:ALA:HA   | 2:665:B:ILE:HD13 | 12       | 0.28          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 8        | 0.28          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 8        | 0.28          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 8        | 0.28          |
| (2,18)   | 1:220:A:LEU:HD21 | 1:221:A:ARG:HG2  | 9        | 0.27          |
| (2,18)   | 1:220:A:LEU:HD22 | 1:221:A:ARG:HG2  | 9        | 0.27          |
| (2,18)   | 1:220:A:LEU:HD23 | 1:221:A:ARG:HG2  | 9        | 0.27          |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 6        | 0.27          |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 6        | 0.27          |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 6        | 0.27          |
| (1,1979) | 2:628:B:LEU:HD21 | 2:630:B:THR:H    | 4        | 0.27          |
| (1,1979) | 2:628:B:LEU:HD22 | 2:630:B:THR:H    | 4        | 0.27          |
| (1,1979) | 2:628:B:LEU:HD23 | 2:630:B:THR:H    | 4        | 0.27          |
| (1,1944) | 2:623:B:VAL:HG11 | 2:623:B:VAL:H    | 16       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1944) | 2:623:B:VAL:HG12 | 2:623:B:VAL:H    | 16       | 0.27          |
| (1,1944) | 2:623:B:VAL:HG13 | 2:623:B:VAL:H    | 16       | 0.27          |
| (1,1873) | 2:608:B:GLU:HB2  | 2:608:B:GLU:H    | 20       | 0.27          |
| (1,1817) | 2:709:B:GLU:HB2  | 2:710:B:ALA:H    | 19       | 0.27          |
| (1,1783) | 2:727:B:LEU:HB2  | 2:727:B:LEU:H    | 8        | 0.27          |
| (1,1759) | 2:697:B:LEU:HD21 | 2:638:B:GLN:HE22 | 17       | 0.27          |
| (1,1759) | 2:697:B:LEU:HD22 | 2:638:B:GLN:HE22 | 17       | 0.27          |
| (1,1759) | 2:697:B:LEU:HD23 | 2:638:B:GLN:HE22 | 17       | 0.27          |
| (1,1759) | 2:697:B:LEU:HD21 | 2:638:B:GLN:HE22 | 19       | 0.27          |
| (1,1759) | 2:697:B:LEU:HD22 | 2:638:B:GLN:HE22 | 19       | 0.27          |
| (1,1759) | 2:697:B:LEU:HD23 | 2:638:B:GLN:HE22 | 19       | 0.27          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD2  | 13       | 0.27          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD2  | 13       | 0.27          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD2  | 13       | 0.27          |
| (1,1354) | 2:716:B:LYS:HD2  | 2:720:B:GLU:HG3  | 15       | 0.27          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 1        | 0.27          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 1        | 0.27          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 1        | 0.27          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 15       | 0.27          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 15       | 0.27          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 15       | 0.27          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD11 | 15       | 0.27          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD12 | 15       | 0.27          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD13 | 15       | 0.27          |
| (1,1004) | 2:712:B:ARG:HD2  | 2:712:B:ARG:HB2  | 15       | 0.27          |
| (1,998)  | 2:695:B:ILE:HA   | 2:698:B:LYS:HD3  | 8        | 0.27          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD21 | 4        | 0.27          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD22 | 4        | 0.27          |
| (1,943)  | 2:641:B:LEU:HA   | 2:644:B:LEU:HD23 | 4        | 0.27          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 2        | 0.27          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 2        | 0.27          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 2        | 0.27          |
| (1,754)  | 2:673:B:ILE:HG21 | 2:707:B:TRP:HE1  | 13       | 0.27          |
| (1,754)  | 2:673:B:ILE:HG22 | 2:707:B:TRP:HE1  | 13       | 0.27          |
| (1,754)  | 2:673:B:ILE:HG23 | 2:707:B:TRP:HE1  | 13       | 0.27          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 5        | 0.27          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 11       | 0.27          |
| (1,619)  | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 2        | 0.27          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 15       | 0.27          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 14       | 0.27          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 6        | 0.27          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 6        | 0.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 6        | 0.27          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 6        | 0.27          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 6        | 0.27          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 6        | 0.27          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 6        | 0.27          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 6        | 0.27          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 6        | 0.27          |
| (1,432) | 2:634:B:LEU:HB3  | 2:701:B:LYS:HE3  | 4        | 0.27          |
| (1,431) | 2:682:B:ILE:HD11 | 2:671:B:GLN:HG3  | 8        | 0.27          |
| (1,431) | 2:682:B:ILE:HD12 | 2:671:B:GLN:HG3  | 8        | 0.27          |
| (1,431) | 2:682:B:ILE:HD13 | 2:671:B:GLN:HG3  | 8        | 0.27          |
| (1,384) | 2:697:B:LEU:HD11 | 2:694:B:PRO:HA   | 2        | 0.27          |
| (1,384) | 2:697:B:LEU:HD12 | 2:694:B:PRO:HA   | 2        | 0.27          |
| (1,384) | 2:697:B:LEU:HD13 | 2:694:B:PRO:HA   | 2        | 0.27          |
| (1,371) | 2:635:B:GLU:HB2  | 2:632:B:ARG:HA   | 15       | 0.27          |
| (1,354) | 2:715:B:ASN:HB2  | 2:712:B:ARG:HA   | 1        | 0.27          |
| (1,256) | 2:658:B:LEU:HD11 | 2:657:B:THR:HG21 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD11 | 2:657:B:THR:HG22 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD11 | 2:657:B:THR:HG23 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD12 | 2:657:B:THR:HG21 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD12 | 2:657:B:THR:HG22 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD12 | 2:657:B:THR:HG23 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD13 | 2:657:B:THR:HG21 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD13 | 2:657:B:THR:HG22 | 4        | 0.27          |
| (1,256) | 2:658:B:LEU:HD13 | 2:657:B:THR:HG23 | 4        | 0.27          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB1  | 9        | 0.27          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB2  | 9        | 0.27          |
| (1,251) | 2:628:B:LEU:HB3  | 2:629:B:ALA:HB3  | 9        | 0.27          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 8        | 0.27          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 20       | 0.27          |
| (1,220) | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 9        | 0.27          |
| (1,209) | 2:691:B:ILE:HB   | 2:691:B:ILE:HG13 | 12       | 0.27          |
| (1,209) | 2:691:B:ILE:HB   | 2:691:B:ILE:HG13 | 14       | 0.27          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 5        | 0.27          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 5        | 0.27          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 5        | 0.27          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 14       | 0.27          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 14       | 0.27          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 14       | 0.27          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG21 | 20       | 0.27          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG22 | 20       | 0.27          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG23 | 20       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,85)   | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 3        | 0.27          |
| (1,85)   | 2:625:B:GLU:HA   | 2:625:B:GLU:HG2  | 6        | 0.27          |
| (1,85)   | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 11       | 0.27          |
| (1,74)   | 2:613:B:CYS:HB2  | 2:612:B:ARG:HB2  | 19       | 0.27          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 3        | 0.27          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 3        | 0.27          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 3        | 0.27          |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD21 | 19       | 0.27          |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD22 | 19       | 0.27          |
| (1,49)   | 2:649:B:GLN:HA   | 2:644:B:LEU:HD23 | 19       | 0.27          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 12       | 0.26          |
| (1,2509) | 1:211:A:LEU:HD21 | 1:211:A:LEU:HA   | 3        | 0.26          |
| (1,2509) | 1:211:A:LEU:HD22 | 1:211:A:LEU:HA   | 3        | 0.26          |
| (1,2509) | 1:211:A:LEU:HD23 | 1:211:A:LEU:HA   | 3        | 0.26          |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 16       | 0.26          |
| (1,1818) | 2:708:B:ARG:HB2  | 2:709:B:GLU:H    | 16       | 0.26          |
| (1,1644) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HG2  | 16       | 0.26          |
| (1,1644) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HG2  | 16       | 0.26          |
| (1,1644) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HG2  | 16       | 0.26          |
| (1,1520) | 2:612:B:ARG:HG3  | 2:612:B:ARG:HA   | 15       | 0.26          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 1        | 0.26          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 2        | 0.26          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 6        | 0.26          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 9        | 0.26          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 18       | 0.26          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 19       | 0.26          |
| (1,697)  | 2:687:B:LYS:HD2  | 2:688:B:ASN:H    | 2        | 0.26          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 13       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 13       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 13       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 18       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 18       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 18       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 19       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 19       | 0.26          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 19       | 0.26          |
| (1,657)  | 1:211:A:LEU:HD11 | 2:673:B:ILE:H    | 2        | 0.26          |
| (1,657)  | 1:211:A:LEU:HD12 | 2:673:B:ILE:H    | 2        | 0.26          |
| (1,657)  | 1:211:A:LEU:HD13 | 2:673:B:ILE:H    | 2        | 0.26          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 20       | 0.26          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 5        | 0.26          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 13       | 0.26          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,444) | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD21 | 5        | 0.26          |
| (1,444) | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD22 | 5        | 0.26          |
| (1,444) | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD23 | 5        | 0.26          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD2  | 1        | 0.26          |
| (1,364) | 2:706:B:GLU:HB2  | 2:706:B:GLU:HA   | 18       | 0.26          |
| (1,298) | 1:207:A:LEU:HG   | 2:710:B:ALA:HB1  | 12       | 0.26          |
| (1,298) | 1:207:A:LEU:HG   | 2:710:B:ALA:HB2  | 12       | 0.26          |
| (1,298) | 1:207:A:LEU:HG   | 2:710:B:ALA:HB3  | 12       | 0.26          |
| (1,242) | 2:692:B:ALA:HB1  | 2:688:B:ASN:HB2  | 11       | 0.26          |
| (1,242) | 2:692:B:ALA:HB2  | 2:688:B:ASN:HB2  | 11       | 0.26          |
| (1,242) | 2:692:B:ALA:HB3  | 2:688:B:ASN:HB2  | 11       | 0.26          |
| (1,226) | 2:608:B:GLU:HG3  | 2:608:B:GLU:HB3  | 7        | 0.26          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD11 | 19       | 0.26          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD12 | 19       | 0.26          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD13 | 19       | 0.26          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 10       | 0.26          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 10       | 0.26          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 10       | 0.26          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 10       | 0.26          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 10       | 0.26          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 10       | 0.26          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 16       | 0.26          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 16       | 0.26          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 1        | 0.26          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 1        | 0.26          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 1        | 0.26          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 19       | 0.26          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 19       | 0.26          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 19       | 0.26          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 12       | 0.26          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 12       | 0.26          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 12       | 0.26          |
| (1,72)  | 2:648:B:GLU:HA   | 2:651:B:LYS:HD2  | 6        | 0.26          |
| (1,14)  | 2:658:B:LEU:HD21 | 2:667:B:ARG:HD3  | 8        | 0.26          |
| (1,14)  | 2:658:B:LEU:HD22 | 2:667:B:ARG:HD3  | 8        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,14)   | 2:658:B:LEU:HD23 | 2:667:B:ARG:HD3  | 8        | 0.26          |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD11 | 16       | 0.25          |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD12 | 16       | 0.25          |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD13 | 16       | 0.25          |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE1  | 12       | 0.25          |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE2  | 12       | 0.25          |
| (1,2572) | 2:677:B:LYS:HE2  | 1:217:A:MET:HE3  | 12       | 0.25          |
| (1,2509) | 1:211:A:LEU:HD21 | 1:211:A:LEU:HA   | 2        | 0.25          |
| (1,2509) | 1:211:A:LEU:HD22 | 1:211:A:LEU:HA   | 2        | 0.25          |
| (1,2509) | 1:211:A:LEU:HD23 | 1:211:A:LEU:HA   | 2        | 0.25          |
| (1,2463) | 2:621:B:ASP:HA   | 2:711:B:GLN:HE22 | 18       | 0.25          |
| (1,2270) | 2:689:B:PRO:HD2  | 2:688:B:ASN:H    | 13       | 0.25          |
| (1,2186) | 2:671:B:GLN:HG2  | 2:675:B:ALA:H    | 19       | 0.25          |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 5        | 0.25          |
| (1,2046) | 2:643:B:ARG:HG2  | 2:643:B:ARG:H    | 5        | 0.25          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 2        | 0.25          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 16       | 0.25          |
| (1,1922) | 2:617:B:ARG:HG2  | 2:620:B:LEU:H    | 20       | 0.25          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 2        | 0.25          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 10       | 0.25          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 18       | 0.25          |
| (1,1783) | 2:727:B:LEU:HB2  | 2:727:B:LEU:H    | 5        | 0.25          |
| (1,1783) | 2:727:B:LEU:HB2  | 2:727:B:LEU:H    | 11       | 0.25          |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD21 | 7        | 0.25          |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD22 | 7        | 0.25          |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD23 | 7        | 0.25          |
| (1,1682) | 2:606:B:ASN:HB2  | 2:610:B:ILE:HG13 | 16       | 0.25          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 7        | 0.25          |
| (1,1623) | 2:622:B:VAL:HG21 | 2:619:B:GLU:HA   | 6        | 0.25          |
| (1,1623) | 2:622:B:VAL:HG22 | 2:619:B:GLU:HA   | 6        | 0.25          |
| (1,1623) | 2:622:B:VAL:HG23 | 2:619:B:GLU:HA   | 6        | 0.25          |
| (1,1286) | 2:701:B:LYS:HD2  | 2:701:B:LYS:HG3  | 16       | 0.25          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 10       | 0.25          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 10       | 0.25          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 10       | 0.25          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 5        | 0.25          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 5        | 0.25          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 5        | 0.25          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 5        | 0.25          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 5        | 0.25          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 5        | 0.25          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 5        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 5        | 0.25          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 5        | 0.25          |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD11 | 3        | 0.25          |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD12 | 3        | 0.25          |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD13 | 3        | 0.25          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 9        | 0.25          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 9        | 0.25          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 9        | 0.25          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD21 | 10       | 0.25          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD22 | 10       | 0.25          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD23 | 10       | 0.25          |
| (1,754)  | 2:703:B:LYS:HB3  | 2:707:B:TRP:HE1  | 14       | 0.25          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 7        | 0.25          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 16       | 0.25          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 16       | 0.25          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 16       | 0.25          |
| (1,672)  | 2:675:B:ALA:HB1  | 2:678:B:ALA:H    | 10       | 0.25          |
| (1,672)  | 2:675:B:ALA:HB2  | 2:678:B:ALA:H    | 10       | 0.25          |
| (1,672)  | 2:675:B:ALA:HB3  | 2:678:B:ALA:H    | 10       | 0.25          |
| (1,609)  | 2:700:B:LEU:HB3  | 2:701:B:LYS:H    | 8        | 0.25          |
| (1,589)  | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 16       | 0.25          |
| (1,589)  | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 16       | 0.25          |
| (1,589)  | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 16       | 0.25          |
| (1,546)  | 2:620:B:LEU:HD21 | 2:620:B:LEU:H    | 3        | 0.25          |
| (1,546)  | 2:620:B:LEU:HD22 | 2:620:B:LEU:H    | 3        | 0.25          |
| (1,546)  | 2:620:B:LEU:HD23 | 2:620:B:LEU:H    | 3        | 0.25          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 6        | 0.25          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 19       | 0.25          |
| (1,434)  | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 19       | 0.25          |
| (1,364)  | 2:640:B:LYS:HB3  | 2:640:B:LYS:HA   | 3        | 0.25          |
| (1,316)  | 2:716:B:LYS:HA   | 2:719:B:ARG:HD3  | 13       | 0.25          |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 2        | 0.25          |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 2        | 0.25          |
| (1,300)  | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 2        | 0.25          |
| (1,300)  | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 2        | 0.25          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 2        | 0.25          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 2        | 0.25          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 2        | 0.25          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 2        | 0.25          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 2        | 0.25          |
| (1,296) | 2:665:B:ILE:HD11 | 2:629:B:ALA:HB1  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD11 | 2:629:B:ALA:HB2  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD11 | 2:629:B:ALA:HB3  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD12 | 2:629:B:ALA:HB1  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD12 | 2:629:B:ALA:HB2  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD12 | 2:629:B:ALA:HB3  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD13 | 2:629:B:ALA:HB1  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD13 | 2:629:B:ALA:HB2  | 12       | 0.25          |
| (1,296) | 2:665:B:ILE:HD13 | 2:629:B:ALA:HB3  | 12       | 0.25          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 13       | 0.25          |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 13       | 0.25          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 13       | 0.25          |
| (1,260) | 2:637:B:ILE:HG21 | 2:653:B:ARG:HG2  | 9        | 0.25          |
| (1,260) | 2:637:B:ILE:HG22 | 2:653:B:ARG:HG2  | 9        | 0.25          |
| (1,260) | 2:637:B:ILE:HG23 | 2:653:B:ARG:HG2  | 9        | 0.25          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 3        | 0.25          |
| (1,220) | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 11       | 0.25          |
| (1,220) | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 12       | 0.25          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD11 | 7        | 0.25          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD12 | 7        | 0.25          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD13 | 7        | 0.25          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD11 | 13       | 0.25          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD12 | 13       | 0.25          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD13 | 13       | 0.25          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG11 | 2        | 0.25          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG12 | 2        | 0.25          |
| (1,159) | 2:697:B:LEU:HG   | 2:693:B:VAL:HG13 | 2        | 0.25          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 2        | 0.25          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 2        | 0.25          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 2        | 0.25          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 4        | 0.25          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 4        | 0.25          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 4        | 0.25          |
| (1,155) | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD11 | 17       | 0.25          |
| (1,155) | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD12 | 17       | 0.25          |
| (1,155) | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD13 | 17       | 0.25          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 14       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 14       | 0.25          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 14       | 0.25          |
| (1,97)   | 2:657:B:THR:HB   | 2:637:B:ILE:HD11 | 19       | 0.25          |
| (1,97)   | 2:657:B:THR:HB   | 2:637:B:ILE:HD12 | 19       | 0.25          |
| (1,97)   | 2:657:B:THR:HB   | 2:637:B:ILE:HD13 | 19       | 0.25          |
| (1,58)   | 2:716:B:LYS:HA   | 2:719:B:ARG:HG3  | 2        | 0.25          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 10       | 0.25          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 10       | 0.25          |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 10       | 0.25          |
| (1,16)   | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD2  | 3        | 0.25          |
| (1,16)   | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD2  | 3        | 0.25          |
| (1,16)   | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD2  | 3        | 0.25          |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 4        | 0.24          |
| (1,2413) | 2:699:B:ARG:HG3  | 2:699:B:ARG:H    | 10       | 0.24          |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 6        | 0.24          |
| (1,2079) | 2:649:B:GLN:HG3  | 2:649:B:GLN:H    | 2        | 0.24          |
| (1,1980) | 2:627:B:ASN:HD21 | 2:631:B:ILE:H    | 12       | 0.24          |
| (1,1921) | 2:724:B:LYS:HG3  | 2:725:B:TYR:H    | 8        | 0.24          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 15       | 0.24          |
| (1,1911) | 2:724:B:LYS:HB2  | 2:724:B:LYS:H    | 9        | 0.24          |
| (1,1852) | 2:701:B:LYS:HD2  | 2:700:B:LEU:H    | 14       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 18       | 0.24          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 18       | 0.24          |
| (1,1682) | 2:606:B:ASN:HB2  | 2:610:B:ILE:HG13 | 7        | 0.24          |
| (1,1682) | 2:606:B:ASN:HB2  | 2:610:B:ILE:HG13 | 8        | 0.24          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 20       | 0.24          |
| (1,1672) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HE3  | 3        | 0.24          |
| (1,1672) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HE3  | 3        | 0.24          |
| (1,1672) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HE3  | 3        | 0.24          |
| (1,1646) | 2:682:B:ILE:HG12 | 2:678:B:ALA:HB1  | 10       | 0.24          |
| (1,1646) | 2:682:B:ILE:HG12 | 2:678:B:ALA:HB2  | 10       | 0.24          |
| (1,1646) | 2:682:B:ILE:HG12 | 2:678:B:ALA:HB3  | 10       | 0.24          |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 3        | 0.24          |
| (1,1559) | 2:716:B:LYS:HG2  | 2:716:B:LYS:HA   | 14       | 0.24          |
| (1,1548) | 2:672:B:ARG:HD2  | 2:672:B:ARG:HA   | 13       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1539) | 2:702:B:MET:HB3  | 2:699:B:ARG:HA   | 3        | 0.24          |
| (1,1286) | 2:701:B:LYS:HD2  | 2:701:B:LYS:HG3  | 7        | 0.24          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 18       | 0.24          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 19       | 0.24          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 7        | 0.24          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 7        | 0.24          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD11 | 2        | 0.24          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD12 | 2        | 0.24          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD13 | 2        | 0.24          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD11 | 14       | 0.24          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD12 | 14       | 0.24          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD13 | 14       | 0.24          |
| (1,698)  | 2:654:B:LEU:HD21 | 2:688:B:ASN:H    | 8        | 0.24          |
| (1,698)  | 2:654:B:LEU:HD22 | 2:688:B:ASN:H    | 8        | 0.24          |
| (1,698)  | 2:654:B:LEU:HD23 | 2:688:B:ASN:H    | 8        | 0.24          |
| (1,698)  | 2:654:B:LEU:HD21 | 2:688:B:ASN:H    | 18       | 0.24          |
| (1,698)  | 2:654:B:LEU:HD22 | 2:688:B:ASN:H    | 18       | 0.24          |
| (1,698)  | 2:654:B:LEU:HD23 | 2:688:B:ASN:H    | 18       | 0.24          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 5        | 0.24          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 5        | 0.24          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 5        | 0.24          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 9        | 0.24          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 9        | 0.24          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 9        | 0.24          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 2        | 0.24          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 7        | 0.24          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 3        | 0.24          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 16       | 0.24          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 19       | 0.24          |
| (1,467)  | 2:726:B:TYR:HB3  | 2:726:B:TYR:H    | 10       | 0.24          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 7        | 0.24          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 7        | 0.24          |
| (1,434)  | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 7        | 0.24          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 7        | 0.24          |
| (1,434)  | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 7        | 0.24          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 7        | 0.24          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 7        | 0.24          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 7        | 0.24          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 7        | 0.24          |
| (1,429) | 2:717:B:VAL:HA   | 2:716:B:LYS:HD2  | 20       | 0.24          |
| (1,388) | 2:694:B:PRO:HB3  | 2:698:B:LYS:HE3  | 19       | 0.24          |
| (1,384) | 2:697:B:LEU:HD11 | 2:694:B:PRO:HA   | 18       | 0.24          |
| (1,384) | 2:697:B:LEU:HD12 | 2:694:B:PRO:HA   | 18       | 0.24          |
| (1,384) | 2:697:B:LEU:HD13 | 2:694:B:PRO:HA   | 18       | 0.24          |
| (1,354) | 2:674:B:TYR:HB3  | 2:671:B:GLN:HA   | 3        | 0.24          |
| (1,265) | 2:697:B:LEU:HD21 | 2:638:B:GLN:HB2  | 4        | 0.24          |
| (1,265) | 2:697:B:LEU:HD22 | 2:638:B:GLN:HB2  | 4        | 0.24          |
| (1,265) | 2:697:B:LEU:HD23 | 2:638:B:GLN:HB2  | 4        | 0.24          |
| (1,232) | 2:712:B:ARG:HA   | 2:711:B:GLN:HG2  | 20       | 0.24          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 2        | 0.24          |
| (1,220) | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 1        | 0.24          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 13       | 0.24          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 16       | 0.24          |
| (1,203) | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 4        | 0.24          |
| (1,203) | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 16       | 0.24          |
| (1,203) | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 20       | 0.24          |
| (1,193) | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG21 | 17       | 0.24          |
| (1,193) | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG22 | 17       | 0.24          |
| (1,193) | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG23 | 17       | 0.24          |
| (1,193) | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG21 | 17       | 0.24          |
| (1,193) | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG22 | 17       | 0.24          |
| (1,193) | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG23 | 17       | 0.24          |
| (1,190) | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG11 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG12 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG13 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG11 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG12 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG13 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG11 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG12 | 15       | 0.24          |
| (1,190) | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG13 | 15       | 0.24          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD11 | 20       | 0.24          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD12 | 20       | 0.24          |
| (1,133) | 2:649:B:GLN:HG2  | 2:644:B:LEU:HD13 | 20       | 0.24          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 11       | 0.24          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 11       | 0.24          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 11       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 19       | 0.24          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 19       | 0.24          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 19       | 0.24          |
| (1,85)   | 2:625:B:GLU:HA   | 2:625:B:GLU:HG2  | 8        | 0.24          |
| (1,85)   | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 14       | 0.24          |
| (1,61)   | 2:629:B:ALA:HA   | 2:632:B:ARG:HG3  | 18       | 0.24          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 20       | 0.24          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 20       | 0.24          |
| (1,49)   | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 20       | 0.24          |
| (2,4)    | 2:690:B:SER:HA   | 2:643:B:ARG:HG3  | 15       | 0.23          |
| (1,2779) | 1:226:A:LEU:HB2  | 1:226:A:LEU:H    | 15       | 0.23          |
| (1,2773) | 1:225:A:LYS:HG2  | 1:225:A:LYS:H    | 6        | 0.23          |
| (1,2673) | 1:206:A:GLN:HG3  | 1:206:A:GLN:H    | 4        | 0.23          |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD11 | 10       | 0.23          |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD12 | 10       | 0.23          |
| (1,2656) | 2:691:B:ILE:HA   | 1:226:A:LEU:HD13 | 10       | 0.23          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 9        | 0.23          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 15       | 0.23          |
| (1,1921) | 2:724:B:LYS:HG3  | 2:725:B:TYR:H    | 14       | 0.23          |
| (1,1891) | 2:612:B:ARG:HB2  | 2:612:B:ARG:H    | 16       | 0.23          |
| (1,1891) | 2:612:B:ARG:HB2  | 2:612:B:ARG:H    | 20       | 0.23          |
| (1,1867) | 2:719:B:ARG:HG2  | 2:720:B:GLU:H    | 1        | 0.23          |
| (1,1719) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE22 | 20       | 0.23          |
| (1,1719) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE22 | 20       | 0.23          |
| (1,1719) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE22 | 20       | 0.23          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE3  | 3        | 0.23          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE3  | 3        | 0.23          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE3  | 3        | 0.23          |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 10       | 0.23          |
| (1,1549) | 2:672:B:ARG:HG2  | 2:672:B:ARG:HA   | 3        | 0.23          |
| (1,1520) | 2:612:B:ARG:HG3  | 2:612:B:ARG:HA   | 7        | 0.23          |
| (1,1520) | 2:612:B:ARG:HG2  | 2:612:B:ARG:HA   | 16       | 0.23          |
| (1,1330) | 2:627:B:ASN:HB2  | 2:631:B:ILE:HG13 | 3        | 0.23          |
| (1,1286) | 2:701:B:LYS:HD2  | 2:701:B:LYS:HG3  | 3        | 0.23          |
| (1,1286) | 2:701:B:LYS:HD2  | 2:701:B:LYS:HG3  | 11       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 8        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 8        | 0.23          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 14       | 0.23          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 14       | 0.23          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG11 | 5        | 0.23          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG12 | 5        | 0.23          |
| (1,1122) | 2:716:B:LYS:HB3  | 2:717:B:VAL:HG13 | 5        | 0.23          |
| (1,997)  | 2:668:B:LYS:HA   | 2:668:B:LYS:HD2  | 13       | 0.23          |
| (1,938)  | 2:720:B:GLU:HA   | 2:724:B:LYS:HG3  | 16       | 0.23          |
| (1,756)  | 2:620:B:LEU:HD21 | 2:707:B:TRP:HE1  | 17       | 0.23          |
| (1,756)  | 2:620:B:LEU:HD22 | 2:707:B:TRP:HE1  | 17       | 0.23          |
| (1,756)  | 2:620:B:LEU:HD23 | 2:707:B:TRP:HE1  | 17       | 0.23          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 15       | 0.23          |
| (1,609)  | 2:700:B:LEU:HB3  | 2:701:B:LYS:H    | 13       | 0.23          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 1        | 0.23          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 12       | 0.23          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 13       | 0.23          |
| (1,535)  | 2:719:B:ARG:HG3  | 2:720:B:GLU:H    | 2        | 0.23          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 4        | 0.23          |
| (1,488)  | 2:706:B:GLU:HA   | 2:709:B:GLU:H    | 20       | 0.23          |
| (1,463)  | 2:720:B:GLU:HA   | 2:721:B:GLN:HE22 | 12       | 0.23          |
| (1,416)  | 1:219:A:ASP:HA   | 2:695:B:ILE:HD11 | 17       | 0.23          |
| (1,416)  | 1:219:A:ASP:HA   | 2:695:B:ILE:HD12 | 17       | 0.23          |
| (1,416)  | 1:219:A:ASP:HA   | 2:695:B:ILE:HD13 | 17       | 0.23          |
| (1,403)  | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD3  | 6        | 0.23          |
| (1,364)  | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 7        | 0.23          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 6        | 0.23          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 6        | 0.23          |
| (1,274)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 6        | 0.23          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 18       | 0.23          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 18       | 0.23          |
| (1,274)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 18       | 0.23          |
| (1,267)  | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD3  | 17       | 0.23          |
| (1,267)  | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD3  | 17       | 0.23          |
| (1,267)  | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD3  | 17       | 0.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,236) | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 10       | 0.23          |
| (1,226) | 2:608:B:GLU:HG3  | 2:608:B:GLU:HB3  | 9        | 0.23          |
| (1,223) | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD2  | 6        | 0.23          |
| (1,223) | 2:728:B:LYS:HG3  | 2:728:B:LYS:HD2  | 7        | 0.23          |
| (1,223) | 2:716:B:LYS:HG3  | 2:716:B:LYS:HD2  | 14       | 0.23          |
| (1,220) | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 2        | 0.23          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 3        | 0.23          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 8        | 0.23          |
| (1,209) | 2:691:B:ILE:HB   | 2:691:B:ILE:HG13 | 17       | 0.23          |
| (1,203) | 2:728:B:LYS:HD2  | 2:728:B:LYS:HG3  | 7        | 0.23          |
| (1,203) | 2:728:B:LYS:HD2  | 2:728:B:LYS:HG2  | 14       | 0.23          |
| (1,203) | 2:728:B:LYS:HD2  | 2:728:B:LYS:HG3  | 19       | 0.23          |
| (1,197) | 2:641:B:LEU:HD11 | 2:649:B:GLN:HA   | 13       | 0.23          |
| (1,197) | 2:641:B:LEU:HD12 | 2:649:B:GLN:HA   | 13       | 0.23          |
| (1,197) | 2:641:B:LEU:HD13 | 2:649:B:GLN:HA   | 13       | 0.23          |
| (1,180) | 2:700:B:LEU:HB3  | 2:631:B:ILE:HG21 | 14       | 0.23          |
| (1,180) | 2:700:B:LEU:HB3  | 2:631:B:ILE:HG22 | 14       | 0.23          |
| (1,180) | 2:700:B:LEU:HB3  | 2:631:B:ILE:HG23 | 14       | 0.23          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG11 | 11       | 0.23          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG12 | 11       | 0.23          |
| (1,158) | 2:689:B:PRO:HB2  | 2:693:B:VAL:HG13 | 11       | 0.23          |
| (1,150) | 2:657:B:THR:HG21 | 2:658:B:LEU:HD11 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG21 | 2:658:B:LEU:HD12 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG21 | 2:658:B:LEU:HD13 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG22 | 2:658:B:LEU:HD11 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG22 | 2:658:B:LEU:HD12 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG22 | 2:658:B:LEU:HD13 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG23 | 2:658:B:LEU:HD11 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG23 | 2:658:B:LEU:HD12 | 12       | 0.23          |
| (1,150) | 2:657:B:THR:HG23 | 2:658:B:LEU:HD13 | 12       | 0.23          |
| (1,122) | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG21 | 7        | 0.23          |
| (1,122) | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG22 | 7        | 0.23          |
| (1,122) | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG23 | 7        | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 3        | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 3        | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 3        | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 9        | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 9        | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 9        | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 16       | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 16       | 0.23          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 16       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,70)   | 2:632:B:ARG:HA   | 2:635:B:GLU:HB2  | 9        | 0.23          |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD3  | 18       | 0.23          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD21 | 5        | 0.23          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD22 | 5        | 0.23          |
| (1,51)   | 2:651:B:LYS:HE2  | 2:644:B:LEU:HD23 | 5        | 0.23          |
| (1,39)   | 2:686:B:ARG:HA   | 2:658:B:LEU:HD11 | 7        | 0.23          |
| (1,39)   | 2:686:B:ARG:HA   | 2:658:B:LEU:HD12 | 7        | 0.23          |
| (1,39)   | 2:686:B:ARG:HA   | 2:658:B:LEU:HD13 | 7        | 0.23          |
| (1,37)   | 2:638:B:GLN:HA   | 2:641:B:LEU:HD21 | 18       | 0.23          |
| (1,37)   | 2:638:B:GLN:HA   | 2:641:B:LEU:HD22 | 18       | 0.23          |
| (1,37)   | 2:638:B:GLN:HA   | 2:641:B:LEU:HD23 | 18       | 0.23          |
| (1,17)   | 2:624:B:LEU:HD21 | 2:708:B:ARG:HD3  | 18       | 0.23          |
| (1,17)   | 2:624:B:LEU:HD22 | 2:708:B:ARG:HD3  | 18       | 0.23          |
| (1,17)   | 2:624:B:LEU:HD23 | 2:708:B:ARG:HD3  | 18       | 0.23          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 9        | 0.22          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 9        | 0.22          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 5        | 0.22          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 8        | 0.22          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 15       | 0.22          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 16       | 0.22          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 17       | 0.22          |
| (1,2574) | 1:221:A:ARG:HD2  | 1:218:A:GLU:HA   | 17       | 0.22          |
| (1,1911) | 2:724:B:LYS:HB3  | 2:724:B:LYS:H    | 8        | 0.22          |
| (1,1838) | 2:615:B:ASP:HB2  | 2:616:B:GLU:H    | 6        | 0.22          |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 4        | 0.22          |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 13       | 0.22          |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 19       | 0.22          |
| (1,1539) | 2:702:B:MET:HB3  | 2:699:B:ARG:HA   | 18       | 0.22          |
| (1,1520) | 2:612:B:ARG:HG2  | 2:612:B:ARG:HA   | 8        | 0.22          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 4        | 0.22          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 9        | 0.22          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 3        | 0.22          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 3        | 0.22          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 3        | 0.22          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD11 | 9        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD12 | 9        | 0.22          |
| (1,1148) | 2:631:B:ILE:HB   | 2:628:B:LEU:HD13 | 9        | 0.22          |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD21 | 2        | 0.22          |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD22 | 2        | 0.22          |
| (1,917)  | 2:649:B:GLN:HB3  | 2:641:B:LEU:HD23 | 2        | 0.22          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD21 | 4        | 0.22          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD22 | 4        | 0.22          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD23 | 4        | 0.22          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD11 | 7        | 0.22          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD12 | 7        | 0.22          |
| (1,906)  | 2:628:B:LEU:HA   | 2:628:B:LEU:HD13 | 7        | 0.22          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD21 | 16       | 0.22          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD22 | 16       | 0.22          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD23 | 16       | 0.22          |
| (1,754)  | 2:673:B:ILE:HG21 | 2:707:B:TRP:HE1  | 10       | 0.22          |
| (1,754)  | 2:673:B:ILE:HG22 | 2:707:B:TRP:HE1  | 10       | 0.22          |
| (1,754)  | 2:673:B:ILE:HG23 | 2:707:B:TRP:HE1  | 10       | 0.22          |
| (1,746)  | 2:706:B:GLU:HG2  | 2:706:B:GLU:H    | 17       | 0.22          |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 5        | 0.22          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 8        | 0.22          |
| (1,589)  | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 17       | 0.22          |
| (1,589)  | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 17       | 0.22          |
| (1,589)  | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 17       | 0.22          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 8        | 0.22          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 15       | 0.22          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 16       | 0.22          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 17       | 0.22          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 18       | 0.22          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 10       | 0.22          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 10       | 0.22          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 10       | 0.22          |
| (1,511)  | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 9        | 0.22          |
| (1,511)  | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 16       | 0.22          |
| (1,403)  | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 10       | 0.22          |
| (1,364)  | 2:686:B:ARG:HB3  | 2:686:B:ARG:HA   | 8        | 0.22          |
| (1,364)  | 2:686:B:ARG:HB3  | 2:686:B:ARG:HA   | 14       | 0.22          |
| (1,282)  | 2:610:B:ILE:HD11 | 2:608:B:GLU:HG2  | 8        | 0.22          |
| (1,282)  | 2:610:B:ILE:HD12 | 2:608:B:GLU:HG2  | 8        | 0.22          |
| (1,282)  | 2:610:B:ILE:HD13 | 2:608:B:GLU:HG2  | 8        | 0.22          |
| (1,269)  | 2:717:B:VAL:HG21 | 2:720:B:GLU:HB2  | 3        | 0.22          |
| (1,269)  | 2:717:B:VAL:HG22 | 2:720:B:GLU:HB2  | 3        | 0.22          |
| (1,269)  | 2:717:B:VAL:HG23 | 2:720:B:GLU:HB2  | 3        | 0.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,267) | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD2  | 13       | 0.22          |
| (1,267) | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD2  | 13       | 0.22          |
| (1,267) | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD2  | 13       | 0.22          |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 15       | 0.22          |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 15       | 0.22          |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 15       | 0.22          |
| (1,226) | 2:608:B:GLU:HG3  | 2:608:B:GLU:HB3  | 18       | 0.22          |
| (1,223) | 2:728:B:LYS:HG3  | 2:728:B:LYS:HD2  | 1        | 0.22          |
| (1,223) | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD3  | 8        | 0.22          |
| (1,223) | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD2  | 9        | 0.22          |
| (1,223) | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD3  | 19       | 0.22          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 10       | 0.22          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 15       | 0.22          |
| (1,203) | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 1        | 0.22          |
| (1,203) | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 6        | 0.22          |
| (1,203) | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 8        | 0.22          |
| (1,193) | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG21 | 20       | 0.22          |
| (1,193) | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG22 | 20       | 0.22          |
| (1,193) | 2:714:B:PHE:HD1  | 2:717:B:VAL:HG23 | 20       | 0.22          |
| (1,193) | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG21 | 20       | 0.22          |
| (1,193) | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG22 | 20       | 0.22          |
| (1,193) | 2:714:B:PHE:HD2  | 2:717:B:VAL:HG23 | 20       | 0.22          |
| (1,174) | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD11 | 2        | 0.22          |
| (1,174) | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD12 | 2        | 0.22          |
| (1,174) | 2:667:B:ARG:HG2  | 2:682:B:ILE:HD13 | 2        | 0.22          |
| (1,126) | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG21 | 3        | 0.22          |
| (1,126) | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG22 | 3        | 0.22          |
| (1,126) | 2:721:B:GLN:HG3  | 2:717:B:VAL:HG23 | 3        | 0.22          |
| (1,97)  | 2:657:B:THR:HB   | 2:637:B:ILE:HD11 | 6        | 0.22          |
| (1,97)  | 2:657:B:THR:HB   | 2:637:B:ILE:HD12 | 6        | 0.22          |
| (1,97)  | 2:657:B:THR:HB   | 2:637:B:ILE:HD13 | 6        | 0.22          |
| (1,63)  | 2:630:B:THR:HA   | 2:634:B:LEU:HG   | 2        | 0.22          |
| (1,63)  | 2:630:B:THR:HA   | 2:634:B:LEU:HG   | 14       | 0.22          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 17       | 0.22          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 17       | 0.22          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 17       | 0.22          |
| (1,19)  | 1:220:A:LEU:HD21 | 2:681:B:ILE:HA   | 15       | 0.22          |
| (1,19)  | 1:220:A:LEU:HD22 | 2:681:B:ILE:HA   | 15       | 0.22          |
| (1,19)  | 1:220:A:LEU:HD23 | 2:681:B:ILE:HA   | 15       | 0.22          |
| (1,16)  | 2:682:B:ILE:HG21 | 2:667:B:ARG:HD3  | 14       | 0.22          |
| (1,16)  | 2:682:B:ILE:HG22 | 2:667:B:ARG:HD3  | 14       | 0.22          |
| (1,16)  | 2:682:B:ILE:HG23 | 2:667:B:ARG:HD3  | 14       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD21 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD22 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG21 | 1:210:A:LEU:HD23 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD21 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD22 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG22 | 1:210:A:LEU:HD23 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD21 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD22 | 7        | 0.21          |
| (2,13)   | 2:673:B:ILE:HG23 | 1:210:A:LEU:HD23 | 7        | 0.21          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 1        | 0.21          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 7        | 0.21          |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 1        | 0.21          |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 1        | 0.21          |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 1        | 0.21          |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 15       | 0.21          |
| (1,1921) | 2:724:B:LYS:HG3  | 2:725:B:TYR:H    | 11       | 0.21          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 12       | 0.21          |
| (1,1838) | 2:615:B:ASP:HB2  | 2:616:B:GLU:H    | 11       | 0.21          |
| (1,1670) | 2:721:B:GLN:HB2  | 2:721:B:GLN:HG3  | 4        | 0.21          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE3  | 8        | 0.21          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE3  | 8        | 0.21          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE3  | 8        | 0.21          |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 16       | 0.21          |
| (1,1559) | 2:716:B:LYS:HG2  | 2:716:B:LYS:HA   | 17       | 0.21          |
| (1,1354) | 2:716:B:LYS:HD3  | 2:720:B:GLU:HG3  | 20       | 0.21          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG3  | 3        | 0.21          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG3  | 10       | 0.21          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 10       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 2        | 0.21          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 11       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 11       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 11       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 11       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 11       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 11       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 11       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 11       | 0.21          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 11       | 0.21          |
| (1,998)  | 2:695:B:ILE:HA   | 2:698:B:LYS:HD3  | 1        | 0.21          |
| (1,967)  | 2:715:B:ASN:HB2  | 2:624:B:LEU:HD21 | 17       | 0.21          |
| (1,967)  | 2:715:B:ASN:HB2  | 2:624:B:LEU:HD22 | 17       | 0.21          |
| (1,967)  | 2:715:B:ASN:HB2  | 2:624:B:LEU:HD23 | 17       | 0.21          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD11 | 17       | 0.21          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD12 | 17       | 0.21          |
| (1,966)  | 2:701:B:LYS:HE3  | 2:697:B:LEU:HD13 | 17       | 0.21          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD21 | 4        | 0.21          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD22 | 4        | 0.21          |
| (1,791)  | 2:684:B:GLY:HA2  | 1:223:A:LEU:HD23 | 4        | 0.21          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD11 | 12       | 0.21          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD12 | 12       | 0.21          |
| (1,788)  | 1:217:A:MET:HA   | 1:223:A:LEU:HD13 | 12       | 0.21          |
| (1,657)  | 2:670:B:LEU:HD21 | 2:673:B:ILE:H    | 13       | 0.21          |
| (1,657)  | 2:670:B:LEU:HD22 | 2:673:B:ILE:H    | 13       | 0.21          |
| (1,657)  | 2:670:B:LEU:HD23 | 2:673:B:ILE:H    | 13       | 0.21          |
| (1,619)  | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 6        | 0.21          |
| (1,609)  | 2:700:B:LEU:HB3  | 2:701:B:LYS:H    | 4        | 0.21          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 2        | 0.21          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 5        | 0.21          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 9        | 0.21          |
| (1,583)  | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 11       | 0.21          |
| (1,562)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 20       | 0.21          |
| (1,562)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 20       | 0.21          |
| (1,562)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 20       | 0.21          |
| (1,534)  | 2:615:B:ASP:HB2  | 2:615:B:ASP:H    | 15       | 0.21          |
| (1,521)  | 2:675:B:ALA:HB1  | 2:677:B:LYS:H    | 9        | 0.21          |
| (1,521)  | 2:675:B:ALA:HB2  | 2:677:B:LYS:H    | 9        | 0.21          |
| (1,521)  | 2:675:B:ALA:HB3  | 2:677:B:LYS:H    | 9        | 0.21          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 11       | 0.21          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 11       | 0.21          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 11       | 0.21          |
| (1,511)  | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 7        | 0.21          |
| (1,488)  | 2:706:B:GLU:HA   | 2:709:B:GLU:H    | 7        | 0.21          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 9        | 0.21          |
| (1,488)  | 2:706:B:GLU:HA   | 2:709:B:GLU:H    | 10       | 0.21          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 12       | 0.21          |
| (1,488)  | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 15       | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,488) | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 17       | 0.21          |
| (1,403) | 2:653:B:ARG:HG2  | 2:653:B:ARG:HD2  | 13       | 0.21          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD3  | 15       | 0.21          |
| (1,403) | 2:653:B:ARG:HG2  | 2:653:B:ARG:HD2  | 18       | 0.21          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD2  | 20       | 0.21          |
| (1,388) | 2:648:B:GLU:HB3  | 2:651:B:LYS:HE2  | 17       | 0.21          |
| (1,364) | 2:686:B:ARG:HB3  | 2:686:B:ARG:HA   | 16       | 0.21          |
| (1,354) | 2:715:B:ASN:HB3  | 2:712:B:ARG:HA   | 4        | 0.21          |
| (1,351) | 2:711:B:GLN:HB3  | 2:708:B:ARG:HA   | 19       | 0.21          |
| (1,266) | 2:658:B:LEU:HD11 | 2:634:B:LEU:HG   | 1        | 0.21          |
| (1,266) | 2:658:B:LEU:HD12 | 2:634:B:LEU:HG   | 1        | 0.21          |
| (1,266) | 2:658:B:LEU:HD13 | 2:634:B:LEU:HG   | 1        | 0.21          |
| (1,236) | 2:709:B:GLU:HB3  | 2:709:B:GLU:HG3  | 6        | 0.21          |
| (1,236) | 2:709:B:GLU:HB3  | 2:709:B:GLU:HG3  | 11       | 0.21          |
| (1,236) | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 20       | 0.21          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 5        | 0.21          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 12       | 0.21          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 13       | 0.21          |
| (1,223) | 2:716:B:LYS:HG3  | 2:716:B:LYS:HD2  | 4        | 0.21          |
| (1,223) | 2:728:B:LYS:HG2  | 2:728:B:LYS:HD3  | 5        | 0.21          |
| (1,223) | 2:716:B:LYS:HG3  | 2:716:B:LYS:HD2  | 10       | 0.21          |
| (1,223) | 2:728:B:LYS:HG2  | 2:728:B:LYS:HD3  | 13       | 0.21          |
| (1,223) | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD2  | 16       | 0.21          |
| (1,223) | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD2  | 20       | 0.21          |
| (1,220) | 2:647:B:GLU:HG3  | 2:647:B:GLU:HB3  | 3        | 0.21          |
| (1,220) | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 5        | 0.21          |
| (1,220) | 2:647:B:GLU:HG3  | 2:647:B:GLU:HB3  | 10       | 0.21          |
| (1,209) | 2:719:B:ARG:HB3  | 2:719:B:ARG:HG2  | 5        | 0.21          |
| (1,209) | 2:719:B:ARG:HB3  | 2:719:B:ARG:HG2  | 6        | 0.21          |
| (1,209) | 2:691:B:ILE:HB   | 2:691:B:ILE:HG13 | 7        | 0.21          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 11       | 0.21          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 19       | 0.21          |
| (1,203) | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG3  | 3        | 0.21          |
| (1,203) | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 5        | 0.21          |
| (1,203) | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 9        | 0.21          |
| (1,203) | 2:640:B:LYS:HD2  | 2:640:B:LYS:HG3  | 10       | 0.21          |
| (1,203) | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 13       | 0.21          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 18       | 0.21          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 18       | 0.21          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 18       | 0.21          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 18       | 0.21          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 18       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,195)  | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 18       | 0.21          |
| (1,190)  | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG11 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG12 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB1  | 2:696:B:VAL:HG13 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG11 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG12 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB2  | 2:696:B:VAL:HG13 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG11 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG12 | 9        | 0.21          |
| (1,190)  | 2:692:B:ALA:HB3  | 2:696:B:VAL:HG13 | 9        | 0.21          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG21 | 14       | 0.21          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG22 | 14       | 0.21          |
| (1,182)  | 2:686:B:ARG:HG2  | 2:682:B:ILE:HG23 | 14       | 0.21          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 13       | 0.21          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 13       | 0.21          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 13       | 0.21          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 16       | 0.21          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 16       | 0.21          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 16       | 0.21          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 14       | 0.21          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 14       | 0.21          |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 14       | 0.21          |
| (1,74)   | 2:613:B:CYS:HB2  | 2:612:B:ARG:HB2  | 15       | 0.21          |
| (1,66)   | 2:687:B:LYS:HA   | 2:687:B:LYS:HD3  | 20       | 0.21          |
| (1,15)   | 2:654:B:LEU:HD21 | 2:686:B:ARG:HD3  | 7        | 0.21          |
| (1,15)   | 2:654:B:LEU:HD22 | 2:686:B:ARG:HD3  | 7        | 0.21          |
| (1,15)   | 2:654:B:LEU:HD23 | 2:686:B:ARG:HD3  | 7        | 0.21          |
| (1,2710) | 1:213:A:ASP:HB2  | 1:214:A:GLU:H    | 8        | 0.2           |
| (1,2694) | 1:210:A:LEU:HB3  | 1:210:A:LEU:H    | 16       | 0.2           |
| (1,2659) | 1:223:A:LEU:HA   | 1:226:A:LEU:HB2  | 13       | 0.2           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD21 | 10       | 0.2           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD22 | 10       | 0.2           |
| (1,2657) | 1:223:A:LEU:HA   | 1:226:A:LEU:HD23 | 10       | 0.2           |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 6        | 0.2           |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 6        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 2        | 0.2           |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 11       | 0.2           |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 18       | 0.2           |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 19       | 0.2           |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 20       | 0.2           |
| (1,2197) | 2:677:B:LYS:HE2  | 2:677:B:LYS:H    | 11       | 0.2           |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 1        | 0.2           |
| (1,2112) | 2:644:B:LEU:HD21 | 2:652:B:PHE:H    | 18       | 0.2           |
| (1,2112) | 2:644:B:LEU:HD22 | 2:652:B:PHE:H    | 18       | 0.2           |
| (1,2112) | 2:644:B:LEU:HD23 | 2:652:B:PHE:H    | 18       | 0.2           |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 5        | 0.2           |
| (1,1904) | 2:615:B:ASP:HA   | 2:616:B:GLU:H    | 2        | 0.2           |
| (1,1891) | 2:612:B:ARG:HB2  | 2:612:B:ARG:H    | 7        | 0.2           |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 8        | 0.2           |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 14       | 0.2           |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB1  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB2  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB3  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB1  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB2  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB3  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB1  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB2  | 7        | 0.2           |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB3  | 7        | 0.2           |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 1        | 0.2           |
| (1,1489) | 2:653:B:ARG:HD2  | 2:687:B:LYS:HA   | 20       | 0.2           |
| (1,1480) | 2:699:B:ARG:HD3  | 2:699:B:ARG:HA   | 16       | 0.2           |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 6        | 0.2           |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 6        | 0.2           |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 6        | 0.2           |
| (1,1289) | 2:689:B:PRO:HB3  | 2:653:B:ARG:HG3  | 19       | 0.2           |
| (1,1286) | 2:701:B:LYS:HD2  | 2:701:B:LYS:HG3  | 5        | 0.2           |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 15       | 0.2           |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD11 | 2        | 0.2           |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD12 | 2        | 0.2           |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD13 | 2        | 0.2           |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 3        | 0.2           |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 3        | 0.2           |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 3        | 0.2           |
| (1,754)  | 2:703:B:LYS:HB3  | 2:707:B:TRP:HE1  | 17       | 0.2           |
| (1,668)  | 2:716:B:LYS:HA   | 2:718:B:TRP:H    | 3        | 0.2           |
| (1,637)  | 2:633:B:VAL:HG21 | 2:658:B:LEU:H    | 8        | 0.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,637) | 2:633:B:VAL:HG22 | 2:658:B:LEU:H    | 8        | 0.2           |
| (1,637) | 2:633:B:VAL:HG23 | 2:658:B:LEU:H    | 8        | 0.2           |
| (1,637) | 2:654:B:LEU:HD21 | 2:658:B:LEU:H    | 13       | 0.2           |
| (1,637) | 2:654:B:LEU:HD22 | 2:658:B:LEU:H    | 13       | 0.2           |
| (1,637) | 2:654:B:LEU:HD23 | 2:658:B:LEU:H    | 13       | 0.2           |
| (1,616) | 2:643:B:ARG:HG3  | 2:643:B:ARG:H    | 14       | 0.2           |
| (1,614) | 2:640:B:LYS:HB3  | 2:642:B:SER:H    | 19       | 0.2           |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 14       | 0.2           |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 19       | 0.2           |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 11       | 0.2           |
| (1,488) | 2:706:B:GLU:HA   | 2:709:B:GLU:H    | 2        | 0.2           |
| (1,488) | 2:619:B:GLU:HA   | 2:620:B:LEU:H    | 8        | 0.2           |
| (1,488) | 2:706:B:GLU:HA   | 2:709:B:GLU:H    | 11       | 0.2           |
| (1,432) | 2:664:B:VAL:HB   | 2:668:B:LYS:HE2  | 5        | 0.2           |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD11 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD12 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD13 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD11 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD12 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD13 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD11 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD12 | 7        | 0.2           |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD13 | 7        | 0.2           |
| (1,403) | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 17       | 0.2           |
| (1,403) | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 19       | 0.2           |
| (1,389) | 2:677:B:LYS:HG2  | 2:677:B:LYS:HE2  | 11       | 0.2           |
| (1,384) | 2:697:B:LEU:HD11 | 2:694:B:PRO:HA   | 3        | 0.2           |
| (1,384) | 2:697:B:LEU:HD12 | 2:694:B:PRO:HA   | 3        | 0.2           |
| (1,384) | 2:697:B:LEU:HD13 | 2:694:B:PRO:HA   | 3        | 0.2           |
| (1,364) | 2:686:B:ARG:HB3  | 2:686:B:ARG:HA   | 5        | 0.2           |
| (1,354) | 2:715:B:ASN:HB2  | 2:712:B:ARG:HA   | 8        | 0.2           |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 9        | 0.2           |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 9        | 0.2           |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 9        | 0.2           |
| (1,267) | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD3  | 15       | 0.2           |
| (1,267) | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD3  | 15       | 0.2           |
| (1,267) | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD3  | 15       | 0.2           |
| (1,266) | 2:631:B:ILE:HD11 | 2:634:B:LEU:HG   | 20       | 0.2           |
| (1,266) | 2:631:B:ILE:HD12 | 2:634:B:LEU:HG   | 20       | 0.2           |
| (1,266) | 2:631:B:ILE:HD13 | 2:634:B:LEU:HG   | 20       | 0.2           |
| (1,242) | 2:692:B:ALA:HB1  | 2:688:B:ASN:HB2  | 10       | 0.2           |
| (1,242) | 2:692:B:ALA:HB2  | 2:688:B:ASN:HB2  | 10       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,242)  | 2:692:B:ALA:HB3  | 2:688:B:ASN:HB2  | 10       | 0.2           |
| (1,236)  | 2:709:B:GLU:HB3  | 2:709:B:GLU:HG3  | 4        | 0.2           |
| (1,236)  | 2:625:B:GLU:HB2  | 2:625:B:GLU:HG2  | 8        | 0.2           |
| (1,226)  | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 4        | 0.2           |
| (1,226)  | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 14       | 0.2           |
| (1,226)  | 2:608:B:GLU:HG3  | 2:608:B:GLU:HB3  | 15       | 0.2           |
| (1,226)  | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 19       | 0.2           |
| (1,223)  | 2:728:B:LYS:HG3  | 2:728:B:LYS:HD2  | 2        | 0.2           |
| (1,223)  | 2:728:B:LYS:HG3  | 2:728:B:LYS:HD2  | 11       | 0.2           |
| (1,203)  | 2:728:B:LYS:HD2  | 2:728:B:LYS:HG3  | 2        | 0.2           |
| (1,203)  | 2:728:B:LYS:HD2  | 2:728:B:LYS:HG3  | 11       | 0.2           |
| (1,203)  | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 17       | 0.2           |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD11 | 8        | 0.2           |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD12 | 8        | 0.2           |
| (1,174)  | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD13 | 8        | 0.2           |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 15       | 0.2           |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 15       | 0.2           |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 15       | 0.2           |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 17       | 0.2           |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 17       | 0.2           |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 17       | 0.2           |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 8        | 0.2           |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 8        | 0.2           |
| (1,103)  | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 8        | 0.2           |
| (1,63)   | 2:630:B:THR:HA   | 2:634:B:LEU:HG   | 20       | 0.2           |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 20       | 0.2           |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 20       | 0.2           |
| (1,51)   | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 20       | 0.2           |
| (1,14)   | 2:658:B:LEU:HD11 | 2:686:B:ARG:HD2  | 20       | 0.2           |
| (1,14)   | 2:658:B:LEU:HD12 | 2:686:B:ARG:HD2  | 20       | 0.2           |
| (1,14)   | 2:658:B:LEU:HD13 | 2:686:B:ARG:HD2  | 20       | 0.2           |
| (1,12)   | 2:718:B:TRP:HZ3  | 2:723:B:GLU:HA   | 3        | 0.2           |
| (1,1)    | 2:614:B:GLU:HG2  | 2:614:B:GLU:HB3  | 17       | 0.2           |
| (1,2779) | 1:226:A:LEU:HB2  | 1:226:A:LEU:H    | 1        | 0.19          |
| (1,2694) | 1:210:A:LEU:HB3  | 1:210:A:LEU:H    | 5        | 0.19          |
| (1,2605) | 1:220:A:LEU:HB3  | 1:220:A:LEU:HD21 | 9        | 0.19          |
| (1,2605) | 1:220:A:LEU:HB3  | 1:220:A:LEU:HD22 | 9        | 0.19          |
| (1,2605) | 1:220:A:LEU:HB3  | 1:220:A:LEU:HD23 | 9        | 0.19          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 4        | 0.19          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD21 | 4        | 0.19          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD22 | 4        | 0.19          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD23 | 4        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2478) | 1:207:A:LEU:HD21 | 1:207:A:LEU:HA   | 4        | 0.19          |
| (1,2478) | 1:207:A:LEU:HD22 | 1:207:A:LEU:HA   | 4        | 0.19          |
| (1,2478) | 1:207:A:LEU:HD23 | 1:207:A:LEU:HA   | 4        | 0.19          |
| (1,2197) | 2:677:B:LYS:HE2  | 2:677:B:LYS:H    | 18       | 0.19          |
| (1,2071) | 2:649:B:GLN:HG3  | 2:648:B:GLU:H    | 2        | 0.19          |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE2  | 5        | 0.19          |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE2  | 5        | 0.19          |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE2  | 5        | 0.19          |
| (1,1480) | 2:699:B:ARG:HD3  | 2:699:B:ARG:HA   | 13       | 0.19          |
| (1,1354) | 2:716:B:LYS:HD3  | 2:720:B:GLU:HG3  | 8        | 0.19          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 6        | 0.19          |
| (1,1312) | 2:698:B:LYS:HB2  | 2:698:B:LYS:HD3  | 1        | 0.19          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 17       | 0.19          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 20       | 0.19          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 17       | 0.19          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 17       | 0.19          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 17       | 0.19          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD11 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD12 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD13 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD11 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD12 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD13 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD11 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD12 | 3        | 0.19          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD13 | 3        | 0.19          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 20       | 0.19          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 20       | 0.19          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 20       | 0.19          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD21 | 6        | 0.19          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD22 | 6        | 0.19          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD23 | 6        | 0.19          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD21 | 6        | 0.19          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD22 | 6        | 0.19          |
| (1,952)  | 2:652:B:PHE:HB3  | 2:644:B:LEU:HD23 | 6        | 0.19          |
| (1,813)  | 1:227:A:LYS:HD3  | 1:228:A:SER:H    | 7        | 0.19          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 14       | 0.19          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 14       | 0.19          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 14       | 0.19          |
| (1,691)  | 2:654:B:LEU:HD21 | 2:686:B:ARG:H    | 15       | 0.19          |
| (1,691)  | 2:654:B:LEU:HD22 | 2:686:B:ARG:H    | 15       | 0.19          |
| (1,691)  | 2:654:B:LEU:HD23 | 2:686:B:ARG:H    | 15       | 0.19          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,690) | 2:685:B:LEU:HG   | 2:686:B:ARG:H    | 10       | 0.19          |
| (1,670) | 2:674:B:TYR:HB3  | 2:678:B:ALA:H    | 10       | 0.19          |
| (1,613) | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 3        | 0.19          |
| (1,589) | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 1        | 0.19          |
| (1,589) | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 1        | 0.19          |
| (1,589) | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 1        | 0.19          |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 3        | 0.19          |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 4        | 0.19          |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 6        | 0.19          |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 10       | 0.19          |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 20       | 0.19          |
| (1,562) | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 4        | 0.19          |
| (1,562) | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 4        | 0.19          |
| (1,562) | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 4        | 0.19          |
| (1,521) | 2:675:B:ALA:HB1  | 2:677:B:LYS:H    | 11       | 0.19          |
| (1,521) | 2:675:B:ALA:HB2  | 2:677:B:LYS:H    | 11       | 0.19          |
| (1,521) | 2:675:B:ALA:HB3  | 2:677:B:LYS:H    | 11       | 0.19          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 2        | 0.19          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 10       | 0.19          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 17       | 0.19          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 20       | 0.19          |
| (1,477) | 2:712:B:ARG:HA   | 2:715:B:ASN:H    | 2        | 0.19          |
| (1,467) | 2:726:B:TYR:HB3  | 2:726:B:TYR:H    | 2        | 0.19          |
| (1,449) | 2:704:B:GLU:HG3  | 2:628:B:LEU:HD21 | 4        | 0.19          |
| (1,449) | 2:704:B:GLU:HG3  | 2:628:B:LEU:HD22 | 4        | 0.19          |
| (1,449) | 2:704:B:GLU:HG3  | 2:628:B:LEU:HD23 | 4        | 0.19          |
| (1,433) | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 12       | 0.19          |
| (1,417) | 2:699:B:ARG:HG3  | 2:673:B:ILE:HD11 | 14       | 0.19          |
| (1,417) | 2:699:B:ARG:HG3  | 2:673:B:ILE:HD12 | 14       | 0.19          |
| (1,417) | 2:699:B:ARG:HG3  | 2:673:B:ILE:HD13 | 14       | 0.19          |
| (1,409) | 2:697:B:LEU:HD11 | 2:697:B:LEU:HA   | 4        | 0.19          |
| (1,409) | 2:697:B:LEU:HD12 | 2:697:B:LEU:HA   | 4        | 0.19          |
| (1,409) | 2:697:B:LEU:HD13 | 2:697:B:LEU:HA   | 4        | 0.19          |
| (1,403) | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 4        | 0.19          |
| (1,394) | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE2  | 18       | 0.19          |
| (1,394) | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE2  | 18       | 0.19          |
| (1,394) | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE2  | 18       | 0.19          |
| (1,349) | 2:687:B:LYS:HD2  | 2:687:B:LYS:HA   | 9        | 0.19          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 1        | 0.19          |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 1        | 0.19          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 1        | 0.19          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 3        | 0.19          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 3        | 0.19          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 3        | 0.19          |
| (1,236) | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 17       | 0.19          |
| (1,236) | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 18       | 0.19          |
| (1,236) | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 19       | 0.19          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 6        | 0.19          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 17       | 0.19          |
| (1,223) | 2:728:B:LYS:HG2  | 2:728:B:LYS:HD3  | 12       | 0.19          |
| (1,220) | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 6        | 0.19          |
| (1,209) | 2:719:B:ARG:HB3  | 2:719:B:ARG:HG2  | 18       | 0.19          |
| (1,203) | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 12       | 0.19          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 6        | 0.19          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 6        | 0.19          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 6        | 0.19          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 6        | 0.19          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 6        | 0.19          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 6        | 0.19          |
| (1,161) | 2:641:B:LEU:HB2  | 2:693:B:VAL:HG11 | 11       | 0.19          |
| (1,161) | 2:641:B:LEU:HB2  | 2:693:B:VAL:HG12 | 11       | 0.19          |
| (1,161) | 2:641:B:LEU:HB2  | 2:693:B:VAL:HG13 | 11       | 0.19          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 1        | 0.19          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 1        | 0.19          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 1        | 0.19          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 19       | 0.19          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 19       | 0.19          |
| (1,138) | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 19       | 0.19          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 10       | 0.19          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 10       | 0.19          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 10       | 0.19          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 16       | 0.19          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 16       | 0.19          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 16       | 0.19          |
| (1,51)  | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD21 | 4        | 0.19          |
| (1,51)  | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD22 | 4        | 0.19          |
| (1,51)  | 2:651:B:LYS:HE3  | 2:644:B:LEU:HD23 | 4        | 0.19          |
| (1,42)  | 2:697:B:LEU:HA   | 2:697:B:LEU:HD11 | 4        | 0.19          |
| (1,42)  | 2:697:B:LEU:HA   | 2:697:B:LEU:HD12 | 4        | 0.19          |
| (1,42)  | 2:697:B:LEU:HA   | 2:697:B:LEU:HD13 | 4        | 0.19          |
| (1,38)  | 2:682:B:ILE:HA   | 2:696:B:VAL:HG11 | 8        | 0.19          |
| (1,38)  | 2:682:B:ILE:HA   | 2:696:B:VAL:HG12 | 8        | 0.19          |
| (1,38)  | 2:682:B:ILE:HA   | 2:696:B:VAL:HG13 | 8        | 0.19          |
| (1,1)   | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB2  | 13       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB3  | 15       | 0.19          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 3        | 0.18          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 3        | 0.18          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 3        | 0.18          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 10       | 0.18          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 13       | 0.18          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG3  | 14       | 0.18          |
| (1,2463) | 2:621:B:ASP:HA   | 2:711:B:GLN:HE22 | 1        | 0.18          |
| (1,2350) | 2:642:B:SER:H    | 2:643:B:ARG:H    | 13       | 0.18          |
| (1,2071) | 2:649:B:GLN:HG3  | 2:648:B:GLU:H    | 14       | 0.18          |
| (1,2061) | 2:644:B:LEU:HB3  | 2:645:B:SER:H    | 12       | 0.18          |
| (1,2027) | 2:701:B:LYS:HE2  | 2:701:B:LYS:H    | 18       | 0.18          |
| (1,1979) | 2:628:B:LEU:HD21 | 2:630:B:THR:H    | 8        | 0.18          |
| (1,1979) | 2:628:B:LEU:HD22 | 2:630:B:THR:H    | 8        | 0.18          |
| (1,1979) | 2:628:B:LEU:HD23 | 2:630:B:THR:H    | 8        | 0.18          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 1        | 0.18          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 3        | 0.18          |
| (1,1559) | 2:716:B:LYS:HG2  | 2:716:B:LYS:HA   | 4        | 0.18          |
| (1,1549) | 2:672:B:ARG:HG2  | 2:672:B:ARG:HA   | 17       | 0.18          |
| (1,1312) | 2:698:B:LYS:HB3  | 2:698:B:LYS:HD2  | 11       | 0.18          |
| (1,1289) | 2:689:B:PRO:HB3  | 2:653:B:ARG:HG3  | 10       | 0.18          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 6        | 0.18          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 14       | 0.18          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 14       | 0.18          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 14       | 0.18          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 8        | 0.18          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 8        | 0.18          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 8        | 0.18          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 14       | 0.18          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 14       | 0.18          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 14       | 0.18          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD11 | 5        | 0.18          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD12 | 5        | 0.18          |
| (1,1056) | 2:667:B:ARG:HD3  | 2:682:B:ILE:HD13 | 5        | 0.18          |
| (1,998)  | 2:695:B:ILE:HA   | 2:698:B:LYS:HD3  | 2        | 0.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD21 | 10       | 0.18          |
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD22 | 10       | 0.18          |
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD23 | 10       | 0.18          |
| (1,803) | 1:218:A:GLU:HB3  | 1:218:A:GLU:H    | 14       | 0.18          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD21 | 14       | 0.18          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD22 | 14       | 0.18          |
| (1,760) | 1:206:A:GLN:HA   | 1:207:A:LEU:HD23 | 14       | 0.18          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 3        | 0.18          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 3        | 0.18          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 3        | 0.18          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 14       | 0.18          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 14       | 0.18          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 14       | 0.18          |
| (1,690) | 2:686:B:ARG:HG3  | 2:686:B:ARG:H    | 17       | 0.18          |
| (1,659) | 1:211:A:LEU:HD11 | 2:674:B:TYR:H    | 4        | 0.18          |
| (1,659) | 1:211:A:LEU:HD12 | 2:674:B:TYR:H    | 4        | 0.18          |
| (1,659) | 1:211:A:LEU:HD13 | 2:674:B:TYR:H    | 4        | 0.18          |
| (1,583) | 2:634:B:LEU:HA   | 2:634:B:LEU:H    | 7        | 0.18          |
| (1,574) | 2:665:B:ILE:HD11 | 2:630:B:THR:H    | 19       | 0.18          |
| (1,574) | 2:665:B:ILE:HD12 | 2:630:B:THR:H    | 19       | 0.18          |
| (1,574) | 2:665:B:ILE:HD13 | 2:630:B:THR:H    | 19       | 0.18          |
| (1,562) | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 13       | 0.18          |
| (1,562) | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 13       | 0.18          |
| (1,562) | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 13       | 0.18          |
| (1,562) | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 16       | 0.18          |
| (1,562) | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 16       | 0.18          |
| (1,562) | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 16       | 0.18          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 3        | 0.18          |
| (1,499) | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 8        | 0.18          |
| (1,467) | 2:726:B:TYR:HB3  | 2:726:B:TYR:H    | 15       | 0.18          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 9        | 0.18          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 9        | 0.18          |
| (1,403) | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 8        | 0.18          |
| (1,403) | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 9        | 0.18          |
| (1,403) | 2:653:B:ARG:HG2  | 2:653:B:ARG:HD2  | 14       | 0.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,396) | 2:632:B:ARG:HG3  | 2:632:B:ARG:HD2  | 6        | 0.18          |
| (1,296) | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB1  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB2  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB3  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB1  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB2  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB3  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB1  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB2  | 18       | 0.18          |
| (1,296) | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB3  | 18       | 0.18          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 8        | 0.18          |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 8        | 0.18          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 8        | 0.18          |
| (1,267) | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD3  | 7        | 0.18          |
| (1,267) | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD3  | 7        | 0.18          |
| (1,267) | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD3  | 7        | 0.18          |
| (1,256) | 2:631:B:ILE:HD11 | 2:630:B:THR:HG21 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD11 | 2:630:B:THR:HG22 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD11 | 2:630:B:THR:HG23 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD12 | 2:630:B:THR:HG21 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD12 | 2:630:B:THR:HG22 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD12 | 2:630:B:THR:HG23 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD13 | 2:630:B:THR:HG21 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD13 | 2:630:B:THR:HG22 | 9        | 0.18          |
| (1,256) | 2:631:B:ILE:HD13 | 2:630:B:THR:HG23 | 9        | 0.18          |
| (1,236) | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 14       | 0.18          |
| (1,234) | 2:648:B:GLU:HG2  | 2:651:B:LYS:HB3  | 8        | 0.18          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 11       | 0.18          |
| (1,223) | 2:728:B:LYS:HG2  | 2:728:B:LYS:HD3  | 18       | 0.18          |
| (1,203) | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 18       | 0.18          |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD21 | 14       | 0.18          |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD22 | 14       | 0.18          |
| (1,169) | 2:673:B:ILE:HG13 | 2:700:B:LEU:HD23 | 14       | 0.18          |
| (1,151) | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD11 | 4        | 0.18          |
| (1,151) | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD12 | 4        | 0.18          |
| (1,151) | 2:637:B:ILE:HG12 | 2:654:B:LEU:HD13 | 4        | 0.18          |
| (1,138) | 2:637:B:ILE:HB   | 2:657:B:THR:HG21 | 12       | 0.18          |
| (1,138) | 2:637:B:ILE:HB   | 2:657:B:THR:HG22 | 12       | 0.18          |
| (1,138) | 2:637:B:ILE:HB   | 2:657:B:THR:HG23 | 12       | 0.18          |
| (1,122) | 2:672:B:ARG:HG2  | 2:623:B:VAL:HG21 | 19       | 0.18          |
| (1,122) | 2:672:B:ARG:HG2  | 2:623:B:VAL:HG22 | 19       | 0.18          |
| (1,122) | 2:672:B:ARG:HG2  | 2:623:B:VAL:HG23 | 19       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 5        | 0.18          |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 5        | 0.18          |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 5        | 0.18          |
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB2  | 6        | 0.18          |
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB2  | 16       | 0.18          |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB1  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB2  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB3  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB1  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB2  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB3  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB1  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB2  | 20       | 0.17          |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB3  | 20       | 0.17          |
| (1,2673) | 1:206:A:GLN:HG3  | 1:206:A:GLN:H    | 3        | 0.17          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 16       | 0.17          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 16       | 0.17          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD21 | 12       | 0.17          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD22 | 12       | 0.17          |
| (1,2516) | 2:699:B:ARG:HB3  | 1:211:A:LEU:HD23 | 12       | 0.17          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 8        | 0.17          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 8        | 0.17          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 8        | 0.17          |
| (1,2305) | 1:210:A:LEU:HD21 | 2:675:B:ALA:H    | 20       | 0.17          |
| (1,2305) | 1:210:A:LEU:HD22 | 2:675:B:ALA:H    | 20       | 0.17          |
| (1,2305) | 1:210:A:LEU:HD23 | 2:675:B:ALA:H    | 20       | 0.17          |
| (1,2197) | 2:677:B:LYS:HE2  | 2:677:B:LYS:H    | 5        | 0.17          |
| (1,2115) | 2:653:B:ARG:HD3  | 2:653:B:ARG:H    | 20       | 0.17          |
| (1,2100) | 2:651:B:LYS:HE3  | 2:651:B:LYS:H    | 12       | 0.17          |
| (1,1759) | 2:697:B:LEU:HD11 | 2:638:B:GLN:HE22 | 4        | 0.17          |
| (1,1759) | 2:697:B:LEU:HD12 | 2:638:B:GLN:HE22 | 4        | 0.17          |
| (1,1759) | 2:697:B:LEU:HD13 | 2:638:B:GLN:HE22 | 4        | 0.17          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB1  | 10       | 0.17          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB2  | 10       | 0.17          |
| (1,1638) | 1:210:A:LEU:HD21 | 2:675:B:ALA:HB3  | 10       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB1  | 10       | 0.17          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB2  | 10       | 0.17          |
| (1,1638) | 1:210:A:LEU:HD22 | 2:675:B:ALA:HB3  | 10       | 0.17          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB1  | 10       | 0.17          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB2  | 10       | 0.17          |
| (1,1638) | 1:210:A:LEU:HD23 | 2:675:B:ALA:HB3  | 10       | 0.17          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2  | 7        | 0.17          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2  | 7        | 0.17          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2  | 7        | 0.17          |
| (1,1596) | 2:696:B:VAL:HB   | 2:693:B:VAL:HA   | 12       | 0.17          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 2        | 0.17          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 2        | 0.17          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 2        | 0.17          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 7        | 0.17          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 7        | 0.17          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 7        | 0.17          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 17       | 0.17          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 18       | 0.17          |
| (1,1289) | 2:689:B:PRO:HB3  | 2:653:B:ARG:HG3  | 11       | 0.17          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD21 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD22 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD23 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD21 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD22 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD23 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD21 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD22 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD23 | 10       | 0.17          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD21 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD22 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD23 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD21 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD22 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD23 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD21 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD22 | 20       | 0.17          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD23 | 20       | 0.17          |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD11 | 20       | 0.17          |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD12 | 20       | 0.17          |
| (1,966)  | 2:701:B:LYS:HE2  | 2:697:B:LEU:HD13 | 20       | 0.17          |
| (1,920)  | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD21 | 13       | 0.17          |
| (1,920)  | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD22 | 13       | 0.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,920) | 2:714:B:PHE:HB2  | 2:620:B:LEU:HD23 | 13       | 0.17          |
| (1,791) | 2:681:B:ILE:HA   | 1:223:A:LEU:HD21 | 20       | 0.17          |
| (1,791) | 2:681:B:ILE:HA   | 1:223:A:LEU:HD22 | 20       | 0.17          |
| (1,791) | 2:681:B:ILE:HA   | 1:223:A:LEU:HD23 | 20       | 0.17          |
| (1,758) | 1:206:A:GLN:HG3  | 1:206:A:GLN:HB3  | 1        | 0.17          |
| (1,758) | 1:206:A:GLN:HG2  | 1:206:A:GLN:HB3  | 10       | 0.17          |
| (1,697) | 2:687:B:LYS:HD3  | 2:688:B:ASN:H    | 20       | 0.17          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 11       | 0.17          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 11       | 0.17          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 11       | 0.17          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 16       | 0.17          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 16       | 0.17          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 16       | 0.17          |
| (1,692) | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 20       | 0.17          |
| (1,692) | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 20       | 0.17          |
| (1,692) | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 20       | 0.17          |
| (1,637) | 2:633:B:VAL:HG21 | 2:658:B:LEU:H    | 7        | 0.17          |
| (1,637) | 2:633:B:VAL:HG22 | 2:658:B:LEU:H    | 7        | 0.17          |
| (1,637) | 2:633:B:VAL:HG23 | 2:658:B:LEU:H    | 7        | 0.17          |
| (1,589) | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 15       | 0.17          |
| (1,589) | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 15       | 0.17          |
| (1,589) | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 15       | 0.17          |
| (1,562) | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 17       | 0.17          |
| (1,562) | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 17       | 0.17          |
| (1,562) | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 17       | 0.17          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 1        | 0.17          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 15       | 0.17          |
| (1,477) | 2:712:B:ARG:HA   | 2:715:B:ASN:H    | 6        | 0.17          |
| (1,467) | 2:725:B:TYR:HB3  | 2:726:B:TYR:H    | 8        | 0.17          |
| (1,463) | 2:720:B:GLU:HA   | 2:721:B:GLN:HE22 | 1        | 0.17          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 18       | 0.17          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 20       | 0.17          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 20       | 0.17          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 20       | 0.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 20       | 0.17          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 20       | 0.17          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 20       | 0.17          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 20       | 0.17          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 20       | 0.17          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 20       | 0.17          |
| (1,415) | 2:703:B:LYS:HB3  | 2:702:B:MET:HE1  | 1        | 0.17          |
| (1,415) | 2:703:B:LYS:HB3  | 2:702:B:MET:HE2  | 1        | 0.17          |
| (1,415) | 2:703:B:LYS:HB3  | 2:702:B:MET:HE3  | 1        | 0.17          |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE1  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE2  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG21 | 2:702:B:MET:HE3  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE1  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE2  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG22 | 2:702:B:MET:HE3  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE1  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE2  | 7        | 0.17          |
| (1,415) | 2:673:B:ILE:HG23 | 2:702:B:MET:HE3  | 7        | 0.17          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD2  | 12       | 0.17          |
| (1,396) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HD3  | 9        | 0.17          |
| (1,365) | 2:712:B:ARG:HB2  | 2:712:B:ARG:HA   | 15       | 0.17          |
| (1,364) | 2:640:B:LYS:HB2  | 2:640:B:LYS:HA   | 12       | 0.17          |
| (1,364) | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 17       | 0.17          |
| (1,349) | 2:687:B:LYS:HD2  | 2:687:B:LYS:HA   | 15       | 0.17          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 19       | 0.17          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 19       | 0.17          |
| (1,296) | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB1  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB2  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG21 | 2:636:B:ALA:HB3  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB1  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB2  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG22 | 2:636:B:ALA:HB3  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB1  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB2  | 16       | 0.17          |
| (1,296) | 2:633:B:VAL:HG23 | 2:636:B:ALA:HB3  | 16       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 4        | 0.17          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 4        | 0.17          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 4        | 0.17          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 4        | 0.17          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 4        | 0.17          |
| (1,274)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 4        | 0.17          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 11       | 0.17          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 11       | 0.17          |
| (1,274)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 11       | 0.17          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 19       | 0.17          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 19       | 0.17          |
| (1,274)  | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 19       | 0.17          |
| (1,236)  | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 2        | 0.17          |
| (1,236)  | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 5        | 0.17          |
| (1,236)  | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 9        | 0.17          |
| (1,236)  | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 13       | 0.17          |
| (1,223)  | 2:728:B:LYS:HG2  | 2:728:B:LYS:HD3  | 15       | 0.17          |
| (1,220)  | 2:705:B:GLU:HG2  | 2:705:B:GLU:HB3  | 4        | 0.17          |
| (1,220)  | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 17       | 0.17          |
| (1,220)  | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 18       | 0.17          |
| (1,213)  | 2:636:B:ALA:HB1  | 2:637:B:ILE:HG13 | 7        | 0.17          |
| (1,213)  | 2:636:B:ALA:HB2  | 2:637:B:ILE:HG13 | 7        | 0.17          |
| (1,213)  | 2:636:B:ALA:HB3  | 2:637:B:ILE:HG13 | 7        | 0.17          |
| (1,211)  | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG3  | 17       | 0.17          |
| (1,209)  | 2:719:B:ARG:HB3  | 2:719:B:ARG:HG2  | 2        | 0.17          |
| (1,203)  | 2:728:B:LYS:HD3  | 2:728:B:LYS:HG2  | 15       | 0.17          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD11 | 16       | 0.17          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD12 | 16       | 0.17          |
| (1,175)  | 2:654:B:LEU:HB3  | 2:637:B:ILE:HD13 | 16       | 0.17          |
| (1,122)  | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG21 | 20       | 0.17          |
| (1,122)  | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG22 | 20       | 0.17          |
| (1,122)  | 2:624:B:LEU:HB2  | 2:623:B:VAL:HG23 | 20       | 0.17          |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 15       | 0.17          |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 15       | 0.17          |
| (1,53)   | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 15       | 0.17          |
| (1,38)   | 2:682:B:ILE:HA   | 2:696:B:VAL:HG11 | 14       | 0.17          |
| (1,38)   | 2:682:B:ILE:HA   | 2:696:B:VAL:HG12 | 14       | 0.17          |
| (1,38)   | 2:682:B:ILE:HA   | 2:696:B:VAL:HG13 | 14       | 0.17          |
| (1,12)   | 2:611:B:TYR:HD1  | 2:614:B:GLU:HA   | 7        | 0.17          |
| (1,12)   | 2:611:B:TYR:HD2  | 2:614:B:GLU:HA   | 7        | 0.17          |
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB2  | 8        | 0.17          |
| (1,2694) | 1:210:A:LEU:HB3  | 1:210:A:LEU:H    | 15       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 16       | 0.16          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 16       | 0.16          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 16       | 0.16          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 20       | 0.16          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 20       | 0.16          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 20       | 0.16          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD21 | 7        | 0.16          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD22 | 7        | 0.16          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD23 | 7        | 0.16          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 15       | 0.16          |
| (1,1921) | 2:724:B:LYS:HG3  | 2:725:B:TYR:H    | 7        | 0.16          |
| (1,1920) | 2:725:B:TYR:HB2  | 2:725:B:TYR:H    | 2        | 0.16          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H    | 7        | 0.16          |
| (1,1672) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HE3  | 20       | 0.16          |
| (1,1672) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HE3  | 20       | 0.16          |
| (1,1672) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HE3  | 20       | 0.16          |
| (1,1600) | 2:648:B:GLU:HG3  | 2:651:B:LYS:HE2  | 6        | 0.16          |
| (1,1549) | 2:672:B:ARG:HG2  | 2:672:B:ARG:HA   | 9        | 0.16          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 15       | 0.16          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 15       | 0.16          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 15       | 0.16          |
| (1,1353) | 2:647:B:GLU:HB2  | 2:647:B:GLU:HG2  | 14       | 0.16          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD11 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD12 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD13 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD11 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD12 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD13 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD11 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD12 | 7        | 0.16          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD13 | 7        | 0.16          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD21 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD22 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD23 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD21 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD22 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD23 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD21 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD22 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD23 | 2        | 0.16          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD21 | 14       | 0.16          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD22 | 14       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD23 | 14       | 0.16          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD21 | 14       | 0.16          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD22 | 14       | 0.16          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD23 | 14       | 0.16          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD21 | 14       | 0.16          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD22 | 14       | 0.16          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD23 | 14       | 0.16          |
| (1,1025) | 2:705:B:GLU:HA   | 2:705:B:GLU:HG2  | 7        | 0.16          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD21 | 14       | 0.16          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD22 | 14       | 0.16          |
| (1,979)  | 2:697:B:LEU:HA   | 2:700:B:LEU:HD23 | 14       | 0.16          |
| (1,945)  | 2:677:B:LYS:HE2  | 2:677:B:LYS:HG2  | 16       | 0.16          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD21 | 18       | 0.16          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD22 | 18       | 0.16          |
| (1,761)  | 2:711:B:GLN:HA   | 1:207:A:LEU:HD23 | 18       | 0.16          |
| (1,698)  | 2:691:B:ILE:HD11 | 2:688:B:ASN:H    | 12       | 0.16          |
| (1,698)  | 2:691:B:ILE:HD12 | 2:688:B:ASN:H    | 12       | 0.16          |
| (1,698)  | 2:691:B:ILE:HD13 | 2:688:B:ASN:H    | 12       | 0.16          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 8        | 0.16          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 8        | 0.16          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 8        | 0.16          |
| (1,562)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 8        | 0.16          |
| (1,562)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 8        | 0.16          |
| (1,562)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 8        | 0.16          |
| (1,562)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 11       | 0.16          |
| (1,562)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 11       | 0.16          |
| (1,562)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 11       | 0.16          |
| (1,536)  | 2:614:B:GLU:HB2  | 2:615:B:ASP:H    | 10       | 0.16          |
| (1,535)  | 2:719:B:ARG:HG3  | 2:720:B:GLU:H    | 6        | 0.16          |
| (1,528)  | 2:611:B:TYR:HB2  | 2:611:B:TYR:H    | 6        | 0.16          |
| (1,514)  | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 7        | 0.16          |
| (1,514)  | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 7        | 0.16          |
| (1,514)  | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 7        | 0.16          |
| (1,511)  | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 19       | 0.16          |
| (1,499)  | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 6        | 0.16          |
| (1,402)  | 2:712:B:ARG:HB2  | 2:712:B:ARG:HD2  | 19       | 0.16          |
| (1,389)  | 2:677:B:LYS:HG2  | 2:677:B:LYS:HE3  | 17       | 0.16          |
| (1,364)  | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 20       | 0.16          |
| (1,354)  | 2:715:B:ASN:HB2  | 2:712:B:ARG:HA   | 7        | 0.16          |
| (1,354)  | 2:715:B:ASN:HB3  | 2:712:B:ARG:HA   | 11       | 0.16          |
| (1,274)  | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 7        | 0.16          |
| (1,274)  | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 7        | 0.16          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 7        | 0.16          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 12       | 0.16          |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 12       | 0.16          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 12       | 0.16          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 20       | 0.16          |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 20       | 0.16          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 20       | 0.16          |
| (1,267) | 2:695:B:ILE:HG21 | 2:698:B:LYS:HD2  | 16       | 0.16          |
| (1,267) | 2:695:B:ILE:HG22 | 2:698:B:LYS:HD2  | 16       | 0.16          |
| (1,267) | 2:695:B:ILE:HG23 | 2:698:B:LYS:HD2  | 16       | 0.16          |
| (1,250) | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB1  | 18       | 0.16          |
| (1,250) | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB2  | 18       | 0.16          |
| (1,250) | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB3  | 18       | 0.16          |
| (1,236) | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 1        | 0.16          |
| (1,211) | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG2  | 3        | 0.16          |
| (1,211) | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG3  | 11       | 0.16          |
| (1,211) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 16       | 0.16          |
| (1,211) | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG3  | 20       | 0.16          |
| (1,197) | 2:644:B:LEU:HD21 | 2:649:B:GLN:HA   | 3        | 0.16          |
| (1,197) | 2:644:B:LEU:HD22 | 2:649:B:GLN:HA   | 3        | 0.16          |
| (1,197) | 2:644:B:LEU:HD23 | 2:649:B:GLN:HA   | 3        | 0.16          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 1        | 0.16          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 1        | 0.16          |
| (1,144) | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD11 | 16       | 0.16          |
| (1,144) | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD12 | 16       | 0.16          |
| (1,144) | 2:654:B:LEU:HB2  | 2:658:B:LEU:HD13 | 16       | 0.16          |
| (1,143) | 2:634:B:LEU:HG   | 2:658:B:LEU:HD11 | 17       | 0.16          |
| (1,143) | 2:634:B:LEU:HG   | 2:658:B:LEU:HD12 | 17       | 0.16          |
| (1,143) | 2:634:B:LEU:HG   | 2:658:B:LEU:HD13 | 17       | 0.16          |
| (1,86)  | 2:614:B:GLU:HA   | 2:614:B:GLU:HG3  | 17       | 0.16          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 6        | 0.16          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 6        | 0.16          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 6        | 0.16          |
| (1,42)  | 2:697:B:LEU:HA   | 2:697:B:LEU:HD11 | 12       | 0.16          |
| (1,42)  | 2:697:B:LEU:HA   | 2:697:B:LEU:HD12 | 12       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,42)   | 2:697:B:LEU:HA   | 2:697:B:LEU:HD13 | 12       | 0.16          |
| (1,12)   | 2:611:B:TYR:HD1  | 2:616:B:GLU:HA   | 4        | 0.16          |
| (1,12)   | 2:611:B:TYR:HD2  | 2:616:B:GLU:HA   | 4        | 0.16          |
| (1,1)    | 2:616:B:GLU:HG2  | 2:616:B:GLU:HB3  | 2        | 0.16          |
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB2  | 19       | 0.16          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 9        | 0.15          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 9        | 0.15          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 9        | 0.15          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 18       | 0.15          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 18       | 0.15          |
| (1,2575) | 1:218:A:GLU:HB3  | 1:218:A:GLU:HG2  | 6        | 0.15          |
| (1,2557) | 1:220:A:LEU:HD21 | 1:217:A:MET:HA   | 9        | 0.15          |
| (1,2557) | 1:220:A:LEU:HD22 | 1:217:A:MET:HA   | 9        | 0.15          |
| (1,2557) | 1:220:A:LEU:HD23 | 1:217:A:MET:HA   | 9        | 0.15          |
| (1,2458) | 2:703:B:LYS:HG3  | 2:707:B:TRP:HE1  | 19       | 0.15          |
| (1,2280) | 2:690:B:SER:HB2  | 2:690:B:SER:H    | 5        | 0.15          |
| (1,2217) | 2:677:B:LYS:HD2  | 2:680:B:ASP:H    | 6        | 0.15          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 3        | 0.15          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 10       | 0.15          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 14       | 0.15          |
| (1,2112) | 2:644:B:LEU:HD21 | 2:652:B:PHE:H    | 5        | 0.15          |
| (1,2112) | 2:644:B:LEU:HD22 | 2:652:B:PHE:H    | 5        | 0.15          |
| (1,2112) | 2:644:B:LEU:HD23 | 2:652:B:PHE:H    | 5        | 0.15          |
| (1,1920) | 2:725:B:TYR:HB2  | 2:725:B:TYR:H    | 8        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 4        | 0.15          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 4        | 0.15          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 13       | 0.15          |
| (1,1623) | 2:622:B:VAL:HG21 | 2:619:B:GLU:HA   | 1        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1623) | 2:622:B:VAL:HG22 | 2:619:B:GLU:HA   | 1        | 0.15          |
| (1,1623) | 2:622:B:VAL:HG23 | 2:619:B:GLU:HA   | 1        | 0.15          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2  | 1        | 0.15          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2  | 1        | 0.15          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2  | 1        | 0.15          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2  | 6        | 0.15          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2  | 6        | 0.15          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2  | 6        | 0.15          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE3  | 13       | 0.15          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE3  | 13       | 0.15          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE3  | 13       | 0.15          |
| (1,1561) | 2:716:B:LYS:HD2  | 2:716:B:LYS:HA   | 7        | 0.15          |
| (1,1415) | 2:687:B:LYS:HG3  | 2:687:B:LYS:HB2  | 7        | 0.15          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 1        | 0.15          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 1        | 0.15          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 1        | 0.15          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 10       | 0.15          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 10       | 0.15          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 10       | 0.15          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 19       | 0.15          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 19       | 0.15          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 19       | 0.15          |
| (1,1353) | 2:647:B:GLU:HB2  | 2:647:B:GLU:HG2  | 19       | 0.15          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 7        | 0.15          |
| (1,1312) | 2:698:B:LYS:HB3  | 2:698:B:LYS:HD2  | 19       | 0.15          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 14       | 0.15          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD11 | 4        | 0.15          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD12 | 4        | 0.15          |
| (1,1284) | 2:708:B:ARG:HG2  | 2:624:B:LEU:HD13 | 4        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD11 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD12 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD13 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD11 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD12 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD13 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD11 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD12 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD13 | 9        | 0.15          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD11 | 16       | 0.15          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD12 | 16       | 0.15          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD13 | 16       | 0.15          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD11 | 16       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD12 | 16       | 0.15          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD13 | 16       | 0.15          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD11 | 16       | 0.15          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD12 | 16       | 0.15          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD13 | 16       | 0.15          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD21 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD22 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD23 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD21 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD22 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD23 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD21 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD22 | 19       | 0.15          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD23 | 19       | 0.15          |
| (1,1080) | 2:699:B:ARG:HA   | 2:702:B:MET:HE1  | 13       | 0.15          |
| (1,1080) | 2:699:B:ARG:HA   | 2:702:B:MET:HE2  | 13       | 0.15          |
| (1,1080) | 2:699:B:ARG:HA   | 2:702:B:MET:HE3  | 13       | 0.15          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 10       | 0.15          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 10       | 0.15          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 10       | 0.15          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 17       | 0.15          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 17       | 0.15          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 17       | 0.15          |
| (1,1004) | 2:712:B:ARG:HD2  | 2:712:B:ARG:HB2  | 8        | 0.15          |
| (1,921)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD11 | 18       | 0.15          |
| (1,921)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD12 | 18       | 0.15          |
| (1,921)  | 2:686:B:ARG:HD2  | 2:658:B:LEU:HD13 | 18       | 0.15          |
| (1,758)  | 1:206:A:GLN:HG2  | 1:206:A:GLN:HB3  | 19       | 0.15          |
| (1,754)  | 2:673:B:ILE:HG21 | 2:707:B:TRP:HE1  | 2        | 0.15          |
| (1,754)  | 2:673:B:ILE:HG22 | 2:707:B:TRP:HE1  | 2        | 0.15          |
| (1,754)  | 2:673:B:ILE:HG23 | 2:707:B:TRP:HE1  | 2        | 0.15          |
| (1,754)  | 2:673:B:ILE:HG21 | 2:707:B:TRP:HE1  | 4        | 0.15          |
| (1,754)  | 2:673:B:ILE:HG22 | 2:707:B:TRP:HE1  | 4        | 0.15          |
| (1,754)  | 2:673:B:ILE:HG23 | 2:707:B:TRP:HE1  | 4        | 0.15          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 1        | 0.15          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 1        | 0.15          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 1        | 0.15          |
| (1,627)  | 2:644:B:LEU:HB3  | 2:649:B:GLN:H    | 2        | 0.15          |
| (1,624)  | 2:647:B:GLU:HB2  | 2:648:B:GLU:H    | 16       | 0.15          |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 9        | 0.15          |
| (1,562)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 5        | 0.15          |
| (1,562)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 5        | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,562) | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 5        | 0.15          |
| (1,534) | 2:655:B:ASP:HB2  | 2:655:B:ASP:H    | 20       | 0.15          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 5        | 0.15          |
| (1,499) | 2:639:B:LYS:HG3  | 2:640:B:LYS:H    | 12       | 0.15          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 10       | 0.15          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 10       | 0.15          |
| (1,424) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HG21 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HG22 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HG23 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HG21 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HG22 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HG23 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HG21 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HG22 | 20       | 0.15          |
| (1,424) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HG23 | 20       | 0.15          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD11 | 1        | 0.15          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD12 | 1        | 0.15          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD13 | 1        | 0.15          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD11 | 15       | 0.15          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD12 | 15       | 0.15          |
| (1,416) | 1:219:A:ASP:HA   | 2:695:B:ILE:HD13 | 15       | 0.15          |
| (1,416) | 1:222:A:THR:HA   | 2:695:B:ILE:HD11 | 20       | 0.15          |
| (1,416) | 1:222:A:THR:HA   | 2:695:B:ILE:HD12 | 20       | 0.15          |
| (1,416) | 1:222:A:THR:HA   | 2:695:B:ILE:HD13 | 20       | 0.15          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD2  | 11       | 0.15          |
| (1,396) | 2:632:B:ARG:HG3  | 2:632:B:ARG:HD2  | 15       | 0.15          |
| (1,371) | 2:635:B:GLU:HB2  | 2:632:B:ARG:HA   | 20       | 0.15          |
| (1,341) | 2:635:B:GLU:HB3  | 2:635:B:GLU:HA   | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB1  | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB2  | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB3  | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB1  | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB2  | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB3  | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB1  | 11       | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,295) | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB2  | 11       | 0.15          |
| (1,295) | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB3  | 11       | 0.15          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 2        | 0.15          |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 2        | 0.15          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 2        | 0.15          |
| (1,266) | 2:631:B:ILE:HD11 | 2:634:B:LEU:HG   | 14       | 0.15          |
| (1,266) | 2:631:B:ILE:HD12 | 2:634:B:LEU:HG   | 14       | 0.15          |
| (1,266) | 2:631:B:ILE:HD13 | 2:634:B:LEU:HG   | 14       | 0.15          |
| (1,249) | 1:211:A:LEU:HB3  | 2:702:B:MET:HE1  | 18       | 0.15          |
| (1,249) | 1:211:A:LEU:HB3  | 2:702:B:MET:HE2  | 18       | 0.15          |
| (1,249) | 1:211:A:LEU:HB3  | 2:702:B:MET:HE3  | 18       | 0.15          |
| (1,236) | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 3        | 0.15          |
| (1,236) | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 12       | 0.15          |
| (1,223) | 2:687:B:LYS:HG2  | 2:687:B:LYS:HD2  | 17       | 0.15          |
| (1,220) | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 7        | 0.15          |
| (1,211) | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG3  | 13       | 0.15          |
| (1,211) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 18       | 0.15          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG21 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG22 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB1  | 2:682:B:ILE:HG23 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG21 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG22 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB2  | 2:682:B:ILE:HG23 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG21 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG22 | 4        | 0.15          |
| (1,182) | 2:679:B:ALA:HB3  | 2:682:B:ILE:HG23 | 4        | 0.15          |
| (1,174) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD11 | 14       | 0.15          |
| (1,174) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD12 | 14       | 0.15          |
| (1,174) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HD13 | 14       | 0.15          |
| (1,143) | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD11 | 15       | 0.15          |
| (1,143) | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD12 | 15       | 0.15          |
| (1,143) | 2:637:B:ILE:HG13 | 2:658:B:LEU:HD13 | 15       | 0.15          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 13       | 0.15          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 13       | 0.15          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 13       | 0.15          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 8        | 0.15          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 8        | 0.15          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 8        | 0.15          |
| (1,13)  | 2:682:B:ILE:HG21 | 2:686:B:ARG:HD3  | 9        | 0.15          |
| (1,13)  | 2:682:B:ILE:HG22 | 2:686:B:ARG:HD3  | 9        | 0.15          |
| (1,13)  | 2:682:B:ILE:HG23 | 2:686:B:ARG:HD3  | 9        | 0.15          |
| (1,1)   | 2:614:B:GLU:HG2  | 2:614:B:GLU:HB3  | 7        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1)    | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB3 | 11       | 0.15          |
| (1,1)    | 2:616:B:GLU:HG2  | 2:616:B:GLU:HB3 | 18       | 0.15          |
| (2,2)    | 2:707:B:TRP:HD1  | 2:624:B:LEU:HA  | 16       | 0.14          |
| (1,2779) | 1:226:A:LEU:HB2  | 1:226:A:LEU:H   | 13       | 0.14          |
| (1,2740) | 1:219:A:ASP:HB2  | 1:219:A:ASP:H   | 9        | 0.14          |
| (1,2704) | 1:212:A:THR:HG21 | 1:212:A:THR:H   | 19       | 0.14          |
| (1,2704) | 1:212:A:THR:HG22 | 1:212:A:THR:H   | 19       | 0.14          |
| (1,2704) | 1:212:A:THR:HG23 | 1:212:A:THR:H   | 19       | 0.14          |
| (1,2478) | 1:207:A:LEU:HD11 | 1:207:A:LEU:HA  | 15       | 0.14          |
| (1,2478) | 1:207:A:LEU:HD12 | 1:207:A:LEU:HA  | 15       | 0.14          |
| (1,2478) | 1:207:A:LEU:HD13 | 1:207:A:LEU:HA  | 15       | 0.14          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H   | 1        | 0.14          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H   | 7        | 0.14          |
| (1,2027) | 2:701:B:LYS:HE2  | 2:701:B:LYS:H   | 10       | 0.14          |
| (1,1918) | 2:724:B:LYS:HA   | 2:725:B:TYR:H   | 14       | 0.14          |
| (1,1891) | 2:612:B:ARG:HB2  | 2:612:B:ARG:H   | 8        | 0.14          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H   | 5        | 0.14          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H   | 8        | 0.14          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H   | 11       | 0.14          |
| (1,1672) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HE3 | 11       | 0.14          |
| (1,1672) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HE3 | 11       | 0.14          |
| (1,1672) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HE3 | 11       | 0.14          |
| (1,1670) | 2:721:B:GLN:HB2  | 2:721:B:GLN:HG3 | 10       | 0.14          |
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE2 | 10       | 0.14          |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE2 | 10       | 0.14          |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE2 | 10       | 0.14          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2 | 9        | 0.14          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2 | 9        | 0.14          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2 | 9        | 0.14          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2 | 12       | 0.14          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2 | 12       | 0.14          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2 | 12       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3 | 3        | 0.14          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3 | 3        | 0.14          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3 | 3        | 0.14          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3 | 9        | 0.14          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3 | 9        | 0.14          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3 | 9        | 0.14          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3 | 11       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3 | 11       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3 | 11       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3 | 16       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 16       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 16       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 20       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 20       | 0.14          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 20       | 0.14          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 20       | 0.14          |
| (1,1351) | 2:716:B:LYS:HE2  | 2:720:B:GLU:HG3  | 2        | 0.14          |
| (1,1286) | 2:701:B:LYS:HD2  | 2:701:B:LYS:HG3  | 2        | 0.14          |
| (1,1286) | 2:701:B:LYS:HD3  | 2:701:B:LYS:HG2  | 8        | 0.14          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 16       | 0.14          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 16       | 0.14          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 16       | 0.14          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD11 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD12 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD13 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD11 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD12 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD13 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD11 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD12 | 5        | 0.14          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD13 | 5        | 0.14          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG21 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG22 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG23 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG21 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG22 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG23 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG21 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG22 | 19       | 0.14          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG23 | 19       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG11 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG12 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG13 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG11 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG12 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG13 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG11 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG12 | 20       | 0.14          |
| (1,1236) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG13 | 20       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD11 | 12       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD12 | 12       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG11 | 2:658:B:LEU:HD13 | 12       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD11 | 12       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD12 | 12       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG12 | 2:658:B:LEU:HD13 | 12       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD11 | 12       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD12 | 12       | 0.14          |
| (1,1153) | 2:633:B:VAL:HG13 | 2:658:B:LEU:HD13 | 12       | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 2        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 2        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 2        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 4        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 4        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 4        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 5        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 5        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 5        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 6        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 6        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 6        | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 13       | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 13       | 0.14          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 13       | 0.14          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD11 | 7        | 0.14          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD12 | 7        | 0.14          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD13 | 7        | 0.14          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD11 | 14       | 0.14          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD12 | 14       | 0.14          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD13 | 14       | 0.14          |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD11 | 5        | 0.14          |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD12 | 5        | 0.14          |
| (1,921)  | 2:686:B:ARG:HD3  | 2:658:B:LEU:HD13 | 5        | 0.14          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 12       | 0.14          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 12       | 0.14          |
| (1,883)  | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 12       | 0.14          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD21 | 15       | 0.14          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD22 | 15       | 0.14          |
| (1,760)  | 1:206:A:GLN:HA   | 1:207:A:LEU:HD23 | 15       | 0.14          |
| (1,758)  | 1:214:A:GLU:HG2  | 1:214:A:GLU:HB3  | 8        | 0.14          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 17       | 0.14          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 17       | 0.14          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 17       | 0.14          |
| (1,619)  | 2:648:B:GLU:HB3  | 2:645:B:SER:H    | 16       | 0.14          |
| (1,613)  | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 9        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,613) | 2:642:B:SER:HB2  | 2:642:B:SER:H    | 19       | 0.14          |
| (1,589) | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 18       | 0.14          |
| (1,589) | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 18       | 0.14          |
| (1,589) | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 18       | 0.14          |
| (1,582) | 2:640:B:LYS:HD2  | 2:640:B:LYS:H    | 11       | 0.14          |
| (1,562) | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 12       | 0.14          |
| (1,562) | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 12       | 0.14          |
| (1,562) | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 12       | 0.14          |
| (1,521) | 2:677:B:LYS:HD3  | 2:677:B:LYS:H    | 18       | 0.14          |
| (1,511) | 2:700:B:LEU:HG   | 2:700:B:LEU:H    | 18       | 0.14          |
| (1,488) | 2:706:B:GLU:HA   | 2:709:B:GLU:H    | 3        | 0.14          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 15       | 0.14          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 15       | 0.14          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD2  | 16       | 0.14          |
| (1,396) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HD3  | 13       | 0.14          |
| (1,365) | 2:712:B:ARG:HB2  | 2:712:B:ARG:HA   | 5        | 0.14          |
| (1,364) | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 19       | 0.14          |
| (1,349) | 2:687:B:LYS:HD2  | 2:687:B:LYS:HA   | 8        | 0.14          |
| (1,320) | 2:618:B:PHE:HB3  | 2:615:B:ASP:HA   | 6        | 0.14          |
| (1,295) | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB1  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB2  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD11 | 2:636:B:ALA:HB3  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB1  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB2  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD12 | 2:636:B:ALA:HB3  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB1  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB2  | 2        | 0.14          |
| (1,295) | 2:637:B:ILE:HD13 | 2:636:B:ALA:HB3  | 2        | 0.14          |
| (1,281) | 2:622:B:VAL:HG11 | 2:619:B:GLU:HG3  | 7        | 0.14          |
| (1,281) | 2:622:B:VAL:HG12 | 2:619:B:GLU:HG3  | 7        | 0.14          |
| (1,281) | 2:622:B:VAL:HG13 | 2:619:B:GLU:HG3  | 7        | 0.14          |
| (1,274) | 2:622:B:VAL:HG11 | 2:623:B:VAL:HB   | 17       | 0.14          |
| (1,274) | 2:622:B:VAL:HG12 | 2:623:B:VAL:HB   | 17       | 0.14          |
| (1,274) | 2:622:B:VAL:HG13 | 2:623:B:VAL:HB   | 17       | 0.14          |
| (1,267) | 2:637:B:ILE:HD11 | 2:640:B:LYS:HD2  | 19       | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,267) | 2:637:B:ILE:HD12 | 2:640:B:LYS:HD2  | 19       | 0.14          |
| (1,267) | 2:637:B:ILE:HD13 | 2:640:B:LYS:HD2  | 19       | 0.14          |
| (1,236) | 2:625:B:GLU:HB3  | 2:625:B:GLU:HG2  | 7        | 0.14          |
| (1,236) | 2:709:B:GLU:HB3  | 2:709:B:GLU:HG3  | 15       | 0.14          |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 9        | 0.14          |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 9        | 0.14          |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 9        | 0.14          |
| (1,226) | 2:608:B:GLU:HG2  | 2:608:B:GLU:HB3  | 10       | 0.14          |
| (1,220) | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 20       | 0.14          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 4        | 0.14          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD21 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD22 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD11 | 2:641:B:LEU:HD23 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD21 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD22 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD12 | 2:641:B:LEU:HD23 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD21 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD22 | 15       | 0.14          |
| (1,188) | 2:658:B:LEU:HD13 | 2:641:B:LEU:HD23 | 15       | 0.14          |
| (1,176) | 2:700:B:LEU:HG   | 2:673:B:ILE:HD11 | 7        | 0.14          |
| (1,176) | 2:700:B:LEU:HG   | 2:673:B:ILE:HD12 | 7        | 0.14          |
| (1,176) | 2:700:B:LEU:HG   | 2:673:B:ILE:HD13 | 7        | 0.14          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG11 | 2        | 0.14          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG12 | 2        | 0.14          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG13 | 2        | 0.14          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 5        | 0.14          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 5        | 0.14          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 5        | 0.14          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG21 | 5        | 0.14          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG22 | 5        | 0.14          |
| (1,126) | 2:720:B:GLU:HG3  | 2:717:B:VAL:HG23 | 5        | 0.14          |
| (1,85)  | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 20       | 0.14          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 1        | 0.14          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 1        | 0.14          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 1        | 0.14          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB1  | 6        | 0.13          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB2  | 6        | 0.13          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB3  | 6        | 0.13          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB1  | 6        | 0.13          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB2  | 6        | 0.13          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB3  | 6        | 0.13          |
| (2,91)  | 1:222:A:THR:HG23 | 2:692:B:ALA:HB1  | 6        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB2  | 6        | 0.13          |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB3  | 6        | 0.13          |
| (1,2694) | 1:210:A:LEU:HB3  | 1:210:A:LEU:H    | 3        | 0.13          |
| (1,2484) | 2:707:B:TRP:HD1  | 1:207:A:LEU:HD11 | 20       | 0.13          |
| (1,2484) | 2:707:B:TRP:HD1  | 1:207:A:LEU:HD12 | 20       | 0.13          |
| (1,2484) | 2:707:B:TRP:HD1  | 1:207:A:LEU:HD13 | 20       | 0.13          |
| (1,2278) | 2:689:B:PRO:HG2  | 2:688:B:ASN:H    | 3        | 0.13          |
| (1,2278) | 2:689:B:PRO:HG2  | 2:688:B:ASN:H    | 9        | 0.13          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 11       | 0.13          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 17       | 0.13          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 19       | 0.13          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 20       | 0.13          |
| (1,2092) | 2:649:B:GLN:HB2  | 2:650:B:ALA:H    | 19       | 0.13          |
| (1,2027) | 2:701:B:LYS:HE2  | 2:701:B:LYS:H    | 3        | 0.13          |
| (1,1993) | 2:633:B:VAL:HG21 | 2:633:B:VAL:H    | 4        | 0.13          |
| (1,1993) | 2:633:B:VAL:HG22 | 2:633:B:VAL:H    | 4        | 0.13          |
| (1,1993) | 2:633:B:VAL:HG23 | 2:633:B:VAL:H    | 4        | 0.13          |
| (1,1921) | 2:724:B:LYS:HG3  | 2:725:B:TYR:H    | 6        | 0.13          |
| (1,1921) | 2:724:B:LYS:HG2  | 2:725:B:TYR:H    | 9        | 0.13          |
| (1,1911) | 2:724:B:LYS:HB3  | 2:724:B:LYS:H    | 13       | 0.13          |
| (1,1904) | 2:615:B:ASP:HA   | 2:616:B:GLU:H    | 3        | 0.13          |
| (1,1873) | 2:608:B:GLU:HB2  | 2:608:B:GLU:H    | 5        | 0.13          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H    | 18       | 0.13          |
| (1,1838) | 2:615:B:ASP:HB2  | 2:616:B:GLU:H    | 7        | 0.13          |
| (1,1778) | 2:726:B:TYR:HA   | 2:727:B:LEU:H    | 16       | 0.13          |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD21 | 8        | 0.13          |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD22 | 8        | 0.13          |
| (1,1717) | 2:711:B:GLN:HG3  | 2:620:B:LEU:HD23 | 8        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 3        | 0.13          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 3        | 0.13          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2  | 10       | 0.13          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2  | 10       | 0.13          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2  | 10       | 0.13          |
| (1,1600) | 2:648:B:GLU:HG3  | 2:651:B:LYS:HE3  | 8        | 0.13          |
| (1,1561) | 2:716:B:LYS:HD2  | 2:716:B:LYS:HA   | 9        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1520) | 2:612:B:ARG:HG3  | 2:612:B:ARG:HA   | 9        | 0.13          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 17       | 0.13          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 17       | 0.13          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 17       | 0.13          |
| (1,1353) | 2:647:B:GLU:HB2  | 2:647:B:GLU:HG3  | 7        | 0.13          |
| (1,1353) | 2:647:B:GLU:HB2  | 2:647:B:GLU:HG3  | 20       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 11       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 11       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 11       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD21 | 2:686:B:ARG:HA   | 18       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD22 | 2:686:B:ARG:HA   | 18       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD23 | 2:686:B:ARG:HA   | 18       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD11 | 2:686:B:ARG:HA   | 20       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD12 | 2:686:B:ARG:HA   | 20       | 0.13          |
| (1,1276) | 2:654:B:LEU:HD13 | 2:686:B:ARG:HA   | 20       | 0.13          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD11 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD12 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD13 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD11 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD12 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD13 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD11 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD12 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD13 | 3        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD11 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD12 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG21 | 2:682:B:ILE:HD13 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD11 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD12 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG22 | 2:682:B:ILE:HD13 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD11 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD12 | 6        | 0.13          |
| (1,1252) | 2:681:B:ILE:HG23 | 2:682:B:ILE:HD13 | 6        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG21 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG22 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG23 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG21 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG22 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG23 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG21 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG22 | 4        | 0.13          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG23 | 4        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD21 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD22 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG21 | 2:634:B:LEU:HD23 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD21 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD22 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG22 | 2:634:B:LEU:HD23 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD21 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD22 | 3        | 0.13          |
| (1,1234) | 2:630:B:THR:HG23 | 2:634:B:LEU:HD23 | 3        | 0.13          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD21 | 5        | 0.13          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD22 | 5        | 0.13          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD23 | 5        | 0.13          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD21 | 16       | 0.13          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD22 | 16       | 0.13          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD23 | 16       | 0.13          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD21 | 11       | 0.13          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD22 | 11       | 0.13          |
| (1,1162) | 2:649:B:GLN:HG3  | 2:644:B:LEU:HD23 | 11       | 0.13          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 7        | 0.13          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 7        | 0.13          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 7        | 0.13          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG21 | 19       | 0.13          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG22 | 19       | 0.13          |
| (1,1076) | 2:666:B:HIS:HA   | 2:665:B:ILE:HG23 | 19       | 0.13          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD11 | 2        | 0.13          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD12 | 2        | 0.13          |
| (1,964)  | 2:634:B:LEU:HA   | 2:634:B:LEU:HD13 | 2        | 0.13          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD21 | 10       | 0.13          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD22 | 10       | 0.13          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD23 | 10       | 0.13          |
| (1,692)  | 2:685:B:LEU:HD11 | 2:686:B:ARG:H    | 10       | 0.13          |
| (1,692)  | 2:685:B:LEU:HD12 | 2:686:B:ARG:H    | 10       | 0.13          |
| (1,692)  | 2:685:B:LEU:HD13 | 2:686:B:ARG:H    | 10       | 0.13          |
| (1,624)  | 2:647:B:GLU:HB2  | 2:648:B:GLU:H    | 17       | 0.13          |
| (1,614)  | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 1        | 0.13          |
| (1,589)  | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 11       | 0.13          |
| (1,589)  | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 11       | 0.13          |
| (1,589)  | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 11       | 0.13          |
| (1,562)  | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 1        | 0.13          |
| (1,562)  | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 1        | 0.13          |
| (1,562)  | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 1        | 0.13          |
| (1,463)  | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 18       | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 16       | 0.13          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 16       | 0.13          |
| (1,433) | 2:716:B:LYS:HB2  | 2:708:B:ARG:HD3  | 19       | 0.13          |
| (1,364) | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 13       | 0.13          |
| (1,319) | 2:687:B:LYS:HA   | 2:653:B:ARG:HD2  | 12       | 0.13          |
| (1,299) | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB1  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB2  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD11 | 2:669:B:ALA:HB3  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB1  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB2  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD12 | 2:669:B:ALA:HB3  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB1  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB2  | 16       | 0.13          |
| (1,299) | 2:700:B:LEU:HD13 | 2:669:B:ALA:HB3  | 16       | 0.13          |
| (1,211) | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG3  | 2        | 0.13          |
| (1,211) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 6        | 0.13          |
| (1,211) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 9        | 0.13          |
| (1,211) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 12       | 0.13          |
| (1,209) | 2:612:B:ARG:HB3  | 2:612:B:ARG:HG2  | 20       | 0.13          |
| (1,192) | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD11 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD12 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD21 | 2:670:B:LEU:HD13 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD11 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD12 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD22 | 2:670:B:LEU:HD13 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD11 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD12 | 11       | 0.13          |
| (1,192) | 2:658:B:LEU:HD23 | 2:670:B:LEU:HD13 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD21 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD22 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD21 | 2:641:B:LEU:HD23 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD21 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD22 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD22 | 2:641:B:LEU:HD23 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD21 | 11       | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD22 | 11       | 0.13          |
| (1,188) | 2:685:B:LEU:HD23 | 2:641:B:LEU:HD23 | 11       | 0.13          |
| (1,179) | 2:697:B:LEU:HG   | 2:631:B:ILE:HG21 | 8        | 0.13          |
| (1,179) | 2:697:B:LEU:HG   | 2:631:B:ILE:HG22 | 8        | 0.13          |
| (1,179) | 2:697:B:LEU:HG   | 2:631:B:ILE:HG23 | 8        | 0.13          |
| (1,133) | 2:638:B:GLN:HG3  | 2:693:B:VAL:HG21 | 7        | 0.13          |
| (1,133) | 2:638:B:GLN:HG3  | 2:693:B:VAL:HG22 | 7        | 0.13          |
| (1,133) | 2:638:B:GLN:HG3  | 2:693:B:VAL:HG23 | 7        | 0.13          |
| (1,95)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HD11 | 13       | 0.13          |
| (1,95)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HD12 | 13       | 0.13          |
| (1,95)  | 2:662:B:SER:HB3  | 2:665:B:ILE:HD13 | 13       | 0.13          |
| (1,85)  | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 1        | 0.13          |
| (1,63)  | 2:630:B:THR:HA   | 2:634:B:LEU:HG   | 3        | 0.13          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD21 | 13       | 0.13          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD22 | 13       | 0.13          |
| (1,53)  | 2:620:B:LEU:HA   | 2:624:B:LEU:HD23 | 13       | 0.13          |
| (1,38)  | 2:682:B:ILE:HA   | 2:696:B:VAL:HG11 | 11       | 0.13          |
| (1,38)  | 2:682:B:ILE:HA   | 2:696:B:VAL:HG12 | 11       | 0.13          |
| (1,38)  | 2:682:B:ILE:HA   | 2:696:B:VAL:HG13 | 11       | 0.13          |
| (1,1)   | 2:614:B:GLU:HG2  | 2:614:B:GLU:HB3  | 1        | 0.13          |
| (1,1)   | 2:723:B:GLU:HG3  | 2:723:B:GLU:HB2  | 12       | 0.13          |
| (1,1)   | 2:616:B:GLU:HG2  | 2:616:B:GLU:HB3  | 14       | 0.13          |
| (1,1)   | 2:616:B:GLU:HG2  | 2:616:B:GLU:HB3  | 20       | 0.13          |
| (3,75)  | 2:702:B:MET:O    | 2:706:B:GLU:H    | 3        | 0.12          |
| (3,27)  | 2:629:B:ALA:O    | 2:633:B:VAL:H    | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB1  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB2  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB3  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB1  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB2  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB3  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG23 | 2:692:B:ALA:HB1  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG23 | 2:692:B:ALA:HB2  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG23 | 2:692:B:ALA:HB3  | 1        | 0.12          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB1  | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB2  | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG21 | 2:692:B:ALA:HB3  | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB1  | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB2  | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG22 | 2:692:B:ALA:HB3  | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG23 | 2:692:B:ALA:HB1  | 7        | 0.12          |
| (2,91)  | 1:222:A:THR:HG23 | 2:692:B:ALA:HB2  | 7        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB3  | 7        | 0.12          |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB1  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB2  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB3  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB1  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB2  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB3  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB1  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB2  | 17       | 0.12          |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB3  | 17       | 0.12          |
| (1,2779) | 1:226:A:LEU:HB2  | 1:226:A:LEU:H    | 19       | 0.12          |
| (1,2749) | 1:221:A:ARG:HG3  | 1:221:A:ARG:H    | 8        | 0.12          |
| (1,2704) | 1:212:A:THR:HG21 | 1:212:A:THR:H    | 3        | 0.12          |
| (1,2704) | 1:212:A:THR:HG22 | 1:212:A:THR:H    | 3        | 0.12          |
| (1,2704) | 1:212:A:THR:HG23 | 1:212:A:THR:H    | 3        | 0.12          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 6        | 0.12          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 6        | 0.12          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 6        | 0.12          |
| (1,2642) | 2:688:B:ASN:HB2  | 1:223:A:LEU:HD21 | 5        | 0.12          |
| (1,2642) | 2:688:B:ASN:HB2  | 1:223:A:LEU:HD22 | 5        | 0.12          |
| (1,2642) | 2:688:B:ASN:HB2  | 1:223:A:LEU:HD23 | 5        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 1        | 0.12          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 15       | 0.12          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 15       | 0.12          |
| (1,2576) | 1:218:A:GLU:HB2  | 1:218:A:GLU:HG3  | 6        | 0.12          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE1  | 14       | 0.12          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE2  | 14       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE3  | 14       | 0.12          |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG21 | 10       | 0.12          |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG22 | 10       | 0.12          |
| (1,2553) | 2:677:B:LYS:HE3  | 1:216:A:ILE:HG23 | 10       | 0.12          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD21 | 6        | 0.12          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD22 | 6        | 0.12          |
| (1,2506) | 2:674:B:TYR:HA   | 1:210:A:LEU:HD23 | 6        | 0.12          |
| (1,2478) | 1:207:A:LEU:HD21 | 1:207:A:LEU:HA   | 16       | 0.12          |
| (1,2478) | 1:207:A:LEU:HD22 | 1:207:A:LEU:HA   | 16       | 0.12          |
| (1,2478) | 1:207:A:LEU:HD23 | 1:207:A:LEU:HA   | 16       | 0.12          |
| (1,2214) | 2:680:B:ASP:HB3  | 2:680:B:ASP:H    | 16       | 0.12          |
| (1,2047) | 2:644:B:LEU:HG   | 2:643:B:ARG:H    | 13       | 0.12          |
| (1,1920) | 2:725:B:TYR:HB2  | 2:725:B:TYR:H    | 12       | 0.12          |
| (1,1918) | 2:724:B:LYS:HA   | 2:725:B:TYR:H    | 4        | 0.12          |
| (1,1891) | 2:612:B:ARG:HB2  | 2:612:B:ARG:H    | 9        | 0.12          |
| (1,1869) | 2:638:B:GLN:HB2  | 2:638:B:GLN:HE21 | 13       | 0.12          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H    | 14       | 0.12          |
| (1,1740) | 2:691:B:ILE:HG12 | 2:688:B:ASN:HD22 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD21 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD22 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD21 | 2:644:B:LEU:HD23 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD21 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD22 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD22 | 2:644:B:LEU:HD23 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD21 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD22 | 1        | 0.12          |
| (1,1707) | 2:641:B:LEU:HD23 | 2:644:B:LEU:HD23 | 1        | 0.12          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 10       | 0.12          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 12       | 0.12          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 18       | 0.12          |
| (1,1672) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HE2  | 4        | 0.12          |
| (1,1672) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HE2  | 4        | 0.12          |
| (1,1672) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HE2  | 4        | 0.12          |
| (1,1614) | 2:682:B:ILE:HD11 | 2:679:B:ALA:HA   | 19       | 0.12          |
| (1,1614) | 2:682:B:ILE:HD12 | 2:679:B:ALA:HA   | 19       | 0.12          |
| (1,1614) | 2:682:B:ILE:HD13 | 2:679:B:ALA:HA   | 19       | 0.12          |
| (1,1611) | 2:693:B:VAL:HB   | 2:694:B:PRO:HD3  | 7        | 0.12          |
| (1,1604) | 2:664:B:VAL:HG11 | 2:668:B:LYS:HE2  | 2        | 0.12          |
| (1,1604) | 2:664:B:VAL:HG12 | 2:668:B:LYS:HE2  | 2        | 0.12          |
| (1,1604) | 2:664:B:VAL:HG13 | 2:668:B:LYS:HE2  | 2        | 0.12          |
| (1,1559) | 2:716:B:LYS:HG2  | 2:716:B:LYS:HA   | 3        | 0.12          |
| (1,1418) | 2:717:B:VAL:HG11 | 2:720:B:GLU:HG2  | 6        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1418) | 2:717:B:VAL:HG12 | 2:720:B:GLU:HG2  | 6        | 0.12          |
| (1,1418) | 2:717:B:VAL:HG13 | 2:720:B:GLU:HG2  | 6        | 0.12          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 4        | 0.12          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 4        | 0.12          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 4        | 0.12          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 18       | 0.12          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 18       | 0.12          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 18       | 0.12          |
| (1,1324) | 2:612:B:ARG:HG2  | 2:612:B:ARG:HB2  | 9        | 0.12          |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB2  | 3        | 0.12          |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB3  | 8        | 0.12          |
| (1,1312) | 2:698:B:LYS:HB2  | 2:698:B:LYS:HD3  | 3        | 0.12          |
| (1,1312) | 2:698:B:LYS:HB3  | 2:698:B:LYS:HD2  | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG21 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG22 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG23 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG21 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG22 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG23 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG21 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG22 | 16       | 0.12          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG23 | 16       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD11 | 2:631:B:ILE:HD11 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD11 | 2:631:B:ILE:HD12 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD11 | 2:631:B:ILE:HD13 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD12 | 2:631:B:ILE:HD11 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD12 | 2:631:B:ILE:HD12 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD12 | 2:631:B:ILE:HD13 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD13 | 2:631:B:ILE:HD11 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD13 | 2:631:B:ILE:HD12 | 17       | 0.12          |
| (1,1204) | 2:700:B:LEU:HD13 | 2:631:B:ILE:HD13 | 17       | 0.12          |
| (1,1202) | 2:701:B:LYS:HD2  | 2:631:B:ILE:HD11 | 12       | 0.12          |
| (1,1202) | 2:701:B:LYS:HD2  | 2:631:B:ILE:HD12 | 12       | 0.12          |
| (1,1202) | 2:701:B:LYS:HD2  | 2:631:B:ILE:HD13 | 12       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD11 | 1        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD12 | 1        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD13 | 1        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD11 | 2        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD12 | 2        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD13 | 2        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD11 | 4        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB   | 2:682:B:ILE:HD12 | 4        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 4        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD11 | 8        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD12 | 8        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 8        | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD11 | 10       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD12 | 10       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 10       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD11 | 11       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD12 | 11       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 11       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD11 | 12       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD12 | 12       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 12       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD11 | 14       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD12 | 14       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 14       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD11 | 15       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD12 | 15       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 15       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD11 | 18       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD12 | 18       | 0.12          |
| (1,1192) | 2:682:B:ILE:HB  | 2:682:B:ILE:HD13 | 18       | 0.12          |
| (1,1168) | 2:624:B:LEU:HB2 | 2:624:B:LEU:HD21 | 12       | 0.12          |
| (1,1168) | 2:624:B:LEU:HB2 | 2:624:B:LEU:HD22 | 12       | 0.12          |
| (1,1168) | 2:624:B:LEU:HB2 | 2:624:B:LEU:HD23 | 12       | 0.12          |
| (1,1162) | 2:649:B:GLN:HG3 | 2:644:B:LEU:HD21 | 9        | 0.12          |
| (1,1162) | 2:649:B:GLN:HG3 | 2:644:B:LEU:HD22 | 9        | 0.12          |
| (1,1162) | 2:649:B:GLN:HG3 | 2:644:B:LEU:HD23 | 9        | 0.12          |
| (1,1154) | 2:654:B:LEU:HB3 | 2:654:B:LEU:HD11 | 1        | 0.12          |
| (1,1154) | 2:654:B:LEU:HB3 | 2:654:B:LEU:HD12 | 1        | 0.12          |
| (1,1154) | 2:654:B:LEU:HB3 | 2:654:B:LEU:HD13 | 1        | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD21 | 11       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD22 | 11       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD23 | 11       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD21 | 18       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD22 | 18       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD23 | 18       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD21 | 20       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD22 | 20       | 0.12          |
| (1,917)  | 2:649:B:GLN:HG2 | 2:641:B:LEU:HD23 | 20       | 0.12          |
| (1,791)  | 2:681:B:ILE:HA  | 1:223:A:LEU:HD21 | 7        | 0.12          |
| (1,791)  | 2:681:B:ILE:HA  | 1:223:A:LEU:HD22 | 7        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,791) | 2:681:B:ILE:HA   | 1:223:A:LEU:HD23 | 7        | 0.12          |
| (1,758) | 1:206:A:GLN:HG2  | 1:206:A:GLN:HB3  | 9        | 0.12          |
| (1,758) | 1:214:A:GLU:HG2  | 1:214:A:GLU:HB3  | 11       | 0.12          |
| (1,758) | 1:206:A:GLN:HG2  | 1:206:A:GLN:HB3  | 14       | 0.12          |
| (1,758) | 1:206:A:GLN:HG2  | 1:206:A:GLN:HB3  | 15       | 0.12          |
| (1,756) | 2:620:B:LEU:HD21 | 2:707:B:TRP:HE1  | 11       | 0.12          |
| (1,756) | 2:620:B:LEU:HD22 | 2:707:B:TRP:HE1  | 11       | 0.12          |
| (1,756) | 2:620:B:LEU:HD23 | 2:707:B:TRP:HE1  | 11       | 0.12          |
| (1,668) | 2:716:B:LYS:HA   | 2:718:B:TRP:H    | 15       | 0.12          |
| (1,624) | 2:647:B:GLU:HB2  | 2:648:B:GLU:H    | 9        | 0.12          |
| (1,605) | 2:643:B:ARG:H    | 2:641:B:LEU:H    | 16       | 0.12          |
| (1,589) | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 9        | 0.12          |
| (1,589) | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 9        | 0.12          |
| (1,589) | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 9        | 0.12          |
| (1,545) | 2:620:B:LEU:HD11 | 2:620:B:LEU:H    | 8        | 0.12          |
| (1,545) | 2:620:B:LEU:HD12 | 2:620:B:LEU:H    | 8        | 0.12          |
| (1,545) | 2:620:B:LEU:HD13 | 2:620:B:LEU:H    | 8        | 0.12          |
| (1,535) | 2:719:B:ARG:HG3  | 2:720:B:GLU:H    | 1        | 0.12          |
| (1,466) | 2:655:B:ASP:HA   | 2:659:B:GLY:H    | 14       | 0.12          |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD11 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD12 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD13 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD11 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD12 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD13 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD11 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD12 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD13 | 4        | 0.12          |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD11 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD12 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD13 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD11 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD12 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD13 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD11 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD12 | 19       | 0.12          |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD13 | 19       | 0.12          |
| (1,420) | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD11 | 15       | 0.12          |
| (1,420) | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD12 | 15       | 0.12          |
| (1,420) | 2:677:B:LYS:HG3  | 2:681:B:ILE:HD13 | 15       | 0.12          |
| (1,403) | 2:653:B:ARG:HG3  | 2:653:B:ARG:HD2  | 2        | 0.12          |
| (1,396) | 2:686:B:ARG:HB2  | 2:686:B:ARG:HD3  | 4        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,394) | 2:644:B:LEU:HD11 | 2:651:B:LYS:HE2  | 9        | 0.12          |
| (1,394) | 2:644:B:LEU:HD12 | 2:651:B:LYS:HE2  | 9        | 0.12          |
| (1,394) | 2:644:B:LEU:HD13 | 2:651:B:LYS:HE2  | 9        | 0.12          |
| (1,364) | 2:704:B:GLU:HB3  | 2:701:B:LYS:HA   | 11       | 0.12          |
| (1,359) | 2:653:B:ARG:HG2  | 2:686:B:ARG:HA   | 9        | 0.12          |
| (1,337) | 2:627:B:ASN:HB2  | 2:628:B:LEU:HA   | 18       | 0.12          |
| (1,315) | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 4        | 0.12          |
| (1,315) | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 17       | 0.12          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 1        | 0.12          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 1        | 0.12          |
| (1,282) | 2:610:B:ILE:HD11 | 2:608:B:GLU:HG3  | 2        | 0.12          |
| (1,282) | 2:610:B:ILE:HD12 | 2:608:B:GLU:HG3  | 2        | 0.12          |
| (1,282) | 2:610:B:ILE:HD13 | 2:608:B:GLU:HG3  | 2        | 0.12          |
| (1,240) | 2:716:B:LYS:HG2  | 2:720:B:GLU:HG2  | 19       | 0.12          |
| (1,236) | 2:709:B:GLU:HB2  | 2:709:B:GLU:HG3  | 16       | 0.12          |
| (1,235) | 2:624:B:LEU:HD11 | 2:704:B:GLU:HG3  | 5        | 0.12          |
| (1,235) | 2:624:B:LEU:HD12 | 2:704:B:GLU:HG3  | 5        | 0.12          |
| (1,235) | 2:624:B:LEU:HD13 | 2:704:B:GLU:HG3  | 5        | 0.12          |
| (1,218) | 2:716:B:LYS:HE2  | 2:716:B:LYS:HD3  | 4        | 0.12          |
| (1,218) | 2:728:B:LYS:HE2  | 2:728:B:LYS:HD3  | 6        | 0.12          |
| (1,211) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 4        | 0.12          |
| (1,211) | 2:667:B:ARG:HB2  | 2:667:B:ARG:HG3  | 19       | 0.12          |
| (1,204) | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD11 | 2        | 0.12          |
| (1,204) | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD12 | 2        | 0.12          |
| (1,204) | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD13 | 2        | 0.12          |
| (1,204) | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD11 | 6        | 0.12          |
| (1,204) | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD12 | 6        | 0.12          |
| (1,204) | 2:708:B:ARG:HB3  | 2:624:B:LEU:HD13 | 6        | 0.12          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD11 | 15       | 0.12          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD12 | 15       | 0.12          |
| (1,204) | 2:704:B:GLU:HG3  | 2:624:B:LEU:HD13 | 15       | 0.12          |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD11 | 7        | 0.12          |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD12 | 7        | 0.12          |
| (1,195) | 1:209:A:TYR:HD1  | 2:620:B:LEU:HD13 | 7        | 0.12          |
| (1,195) | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD11 | 7        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,195) | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD12 | 7        | 0.12          |
| (1,195) | 1:209:A:TYR:HD2  | 2:620:B:LEU:HD13 | 7        | 0.12          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD21 | 20       | 0.12          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD22 | 20       | 0.12          |
| (1,195) | 1:209:A:TYR:HD1  | 2:624:B:LEU:HD23 | 20       | 0.12          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD21 | 20       | 0.12          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD22 | 20       | 0.12          |
| (1,195) | 1:209:A:TYR:HD2  | 2:624:B:LEU:HD23 | 20       | 0.12          |
| (1,182) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HG21 | 6        | 0.12          |
| (1,182) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HG22 | 6        | 0.12          |
| (1,182) | 2:670:B:LEU:HB2  | 2:682:B:ILE:HG23 | 6        | 0.12          |
| (1,176) | 2:700:B:LEU:HG   | 2:673:B:ILE:HD11 | 1        | 0.12          |
| (1,176) | 2:700:B:LEU:HG   | 2:673:B:ILE:HD12 | 1        | 0.12          |
| (1,176) | 2:700:B:LEU:HG   | 2:673:B:ILE:HD13 | 1        | 0.12          |
| (1,170) | 2:634:B:LEU:HG   | 2:700:B:LEU:HD21 | 14       | 0.12          |
| (1,170) | 2:634:B:LEU:HG   | 2:700:B:LEU:HD22 | 14       | 0.12          |
| (1,170) | 2:634:B:LEU:HG   | 2:700:B:LEU:HD23 | 14       | 0.12          |
| (1,169) | 2:670:B:LEU:HB2  | 2:700:B:LEU:HD21 | 13       | 0.12          |
| (1,169) | 2:670:B:LEU:HB2  | 2:700:B:LEU:HD22 | 13       | 0.12          |
| (1,169) | 2:670:B:LEU:HB2  | 2:700:B:LEU:HD23 | 13       | 0.12          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG11 | 12       | 0.12          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG12 | 12       | 0.12          |
| (1,131) | 2:672:B:ARG:HD3  | 2:623:B:VAL:HG13 | 12       | 0.12          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG21 | 12       | 0.12          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG22 | 12       | 0.12          |
| (1,129) | 2:658:B:LEU:HB3  | 2:633:B:VAL:HG23 | 12       | 0.12          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG21 | 2        | 0.12          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG22 | 2        | 0.12          |
| (1,103) | 1:218:A:GLU:HB3  | 2:695:B:ILE:HG23 | 2        | 0.12          |
| (1,85)  | 2:709:B:GLU:HA   | 2:709:B:GLU:HG2  | 5        | 0.12          |
| (1,63)  | 2:630:B:THR:HA   | 2:634:B:LEU:HG   | 19       | 0.12          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD11 | 2        | 0.12          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD12 | 2        | 0.12          |
| (1,49)  | 2:690:B:SER:HB2  | 2:641:B:LEU:HD13 | 2        | 0.12          |
| (1,13)  | 2:682:B:ILE:HG21 | 2:686:B:ARG:HD3  | 5        | 0.12          |
| (1,13)  | 2:682:B:ILE:HG22 | 2:686:B:ARG:HD3  | 5        | 0.12          |
| (1,13)  | 2:682:B:ILE:HG23 | 2:686:B:ARG:HD3  | 5        | 0.12          |
| (1,1)   | 2:616:B:GLU:HG2  | 2:616:B:GLU:HB3  | 3        | 0.12          |
| (1,1)   | 2:616:B:GLU:HG2  | 2:616:B:GLU:HB3  | 5        | 0.12          |
| (3,89)  | 2:714:B:PHE:O    | 2:718:B:TRP:H    | 3        | 0.11          |
| (3,81)  | 2:705:B:GLU:O    | 2:709:B:GLU:H    | 4        | 0.11          |
| (3,69)  | 2:699:B:ARG:O    | 2:703:B:LYS:H    | 20       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,57)   | 2:668:B:LYS:O    | 2:672:B:ARG:H    | 11       | 0.11          |
| (3,45)   | 2:646:B:ALA:O    | 2:650:B:ALA:H    | 11       | 0.11          |
| (3,1)    | 2:616:B:GLU:O    | 2:620:B:LEU:H    | 10       | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 1        | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 1        | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 1        | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 15       | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 15       | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 15       | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD21 | 19       | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD22 | 19       | 0.11          |
| (1,2643) | 2:691:B:ILE:HA   | 1:223:A:LEU:HD23 | 19       | 0.11          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 2        | 0.11          |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 2        | 0.11          |
| (1,2598) | 2:680:B:ASP:HA   | 1:220:A:LEU:HD11 | 20       | 0.11          |
| (1,2598) | 2:680:B:ASP:HA   | 1:220:A:LEU:HD12 | 20       | 0.11          |
| (1,2598) | 2:680:B:ASP:HA   | 1:220:A:LEU:HD13 | 20       | 0.11          |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD11 | 12       | 0.11          |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD12 | 12       | 0.11          |
| (1,2590) | 2:677:B:LYS:HB3  | 1:220:A:LEU:HD13 | 12       | 0.11          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE1  | 13       | 0.11          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE2  | 13       | 0.11          |
| (1,2572) | 2:677:B:LYS:HE3  | 1:217:A:MET:HE3  | 13       | 0.11          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD21 | 18       | 0.11          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD22 | 18       | 0.11          |
| (1,2515) | 2:699:B:ARG:HD3  | 1:211:A:LEU:HD23 | 18       | 0.11          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD21 | 13       | 0.11          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD22 | 13       | 0.11          |
| (1,2491) | 1:209:A:TYR:HD1  | 1:207:A:LEU:HD23 | 13       | 0.11          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD21 | 13       | 0.11          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD22 | 13       | 0.11          |
| (1,2491) | 1:209:A:TYR:HD2  | 1:207:A:LEU:HD23 | 13       | 0.11          |
| (1,2478) | 1:207:A:LEU:HD11 | 1:207:A:LEU:HA   | 13       | 0.11          |
| (1,2478) | 1:207:A:LEU:HD12 | 1:207:A:LEU:HA   | 13       | 0.11          |
| (1,2478) | 1:207:A:LEU:HD13 | 1:207:A:LEU:HA   | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2471) | 1:206:A:GLN:HG2  | 1:206:A:GLN:HA   | 11       | 0.11          |
| (1,2312) | 2:616:B:GLU:HG3  | 2:616:B:GLU:H    | 7        | 0.11          |
| (1,2304) | 2:717:B:VAL:HG21 | 2:721:B:GLN:HE21 | 19       | 0.11          |
| (1,2304) | 2:717:B:VAL:HG22 | 2:721:B:GLN:HE21 | 19       | 0.11          |
| (1,2304) | 2:717:B:VAL:HG23 | 2:721:B:GLN:HE21 | 19       | 0.11          |
| (1,2280) | 2:690:B:SER:HB2  | 2:690:B:SER:H    | 3        | 0.11          |
| (1,2278) | 2:689:B:PRO:HG2  | 2:688:B:ASN:H    | 1        | 0.11          |
| (1,2130) | 2:727:B:LEU:HA   | 2:728:B:LYS:H    | 19       | 0.11          |
| (1,2046) | 2:643:B:ARG:HG2  | 2:643:B:ARG:H    | 19       | 0.11          |
| (1,1980) | 2:627:B:ASN:HD21 | 2:631:B:ILE:H    | 3        | 0.11          |
| (1,1904) | 2:615:B:ASP:HA   | 2:616:B:GLU:H    | 19       | 0.11          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H    | 2        | 0.11          |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H    | 16       | 0.11          |
| (1,1838) | 2:615:B:ASP:HB2  | 2:616:B:GLU:H    | 16       | 0.11          |
| (1,1678) | 2:708:B:ARG:HB2  | 2:708:B:ARG:HD3  | 4        | 0.11          |
| (1,1561) | 2:716:B:LYS:HD2  | 2:716:B:LYS:HA   | 18       | 0.11          |
| (1,1559) | 2:716:B:LYS:HG2  | 2:716:B:LYS:HA   | 16       | 0.11          |
| (1,1520) | 2:612:B:ARG:HG3  | 2:612:B:ARG:HA   | 20       | 0.11          |
| (1,1415) | 2:687:B:LYS:HG3  | 2:687:B:LYS:HB2  | 11       | 0.11          |
| (1,1403) | 2:664:B:VAL:HG21 | 2:668:B:LYS:HD3  | 8        | 0.11          |
| (1,1403) | 2:664:B:VAL:HG22 | 2:668:B:LYS:HD3  | 8        | 0.11          |
| (1,1403) | 2:664:B:VAL:HG23 | 2:668:B:LYS:HD3  | 8        | 0.11          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 14       | 0.11          |
| (1,1352) | 2:647:B:GLU:HB3  | 2:647:B:GLU:HG2  | 19       | 0.11          |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB3  | 6        | 0.11          |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB3  | 11       | 0.11          |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB3  | 13       | 0.11          |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB2  | 14       | 0.11          |
| (1,1314) | 2:709:B:GLU:HG3  | 2:709:B:GLU:HB2  | 20       | 0.11          |
| (1,1262) | 2:674:B:TYR:HD1  | 2:670:B:LEU:HD11 | 8        | 0.11          |
| (1,1262) | 2:674:B:TYR:HD1  | 2:670:B:LEU:HD12 | 8        | 0.11          |
| (1,1262) | 2:674:B:TYR:HD1  | 2:670:B:LEU:HD13 | 8        | 0.11          |
| (1,1262) | 2:674:B:TYR:HD2  | 2:670:B:LEU:HD11 | 8        | 0.11          |
| (1,1262) | 2:674:B:TYR:HD2  | 2:670:B:LEU:HD12 | 8        | 0.11          |
| (1,1262) | 2:674:B:TYR:HD2  | 2:670:B:LEU:HD13 | 8        | 0.11          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG21 | 12       | 0.11          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG22 | 12       | 0.11          |
| (1,1237) | 2:681:B:ILE:HG21 | 2:696:B:VAL:HG23 | 12       | 0.11          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG21 | 12       | 0.11          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG22 | 12       | 0.11          |
| (1,1237) | 2:681:B:ILE:HG22 | 2:696:B:VAL:HG23 | 12       | 0.11          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG21 | 12       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG22 | 12       | 0.11          |
| (1,1237) | 2:681:B:ILE:HG23 | 2:696:B:VAL:HG23 | 12       | 0.11          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD21 | 4        | 0.11          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD22 | 4        | 0.11          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD23 | 4        | 0.11          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD21 | 19       | 0.11          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD22 | 19       | 0.11          |
| (1,1168) | 2:624:B:LEU:HB2  | 2:624:B:LEU:HD23 | 19       | 0.11          |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD11 | 7        | 0.11          |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD12 | 7        | 0.11          |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD13 | 7        | 0.11          |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD11 | 9        | 0.11          |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD12 | 9        | 0.11          |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD13 | 9        | 0.11          |
| (1,1026) | 2:706:B:GLU:HA   | 2:709:B:GLU:HG2  | 6        | 0.11          |
| (1,958)  | 2:644:B:LEU:HA   | 2:644:B:LEU:HD21 | 15       | 0.11          |
| (1,958)  | 2:644:B:LEU:HA   | 2:644:B:LEU:HD22 | 15       | 0.11          |
| (1,958)  | 2:644:B:LEU:HA   | 2:644:B:LEU:HD23 | 15       | 0.11          |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD11 | 14       | 0.11          |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD12 | 14       | 0.11          |
| (1,955)  | 2:631:B:ILE:HA   | 2:634:B:LEU:HD13 | 14       | 0.11          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD21 | 12       | 0.11          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD22 | 12       | 0.11          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD23 | 12       | 0.11          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD21 | 16       | 0.11          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD22 | 16       | 0.11          |
| (1,917)  | 2:649:B:GLN:HG2  | 2:641:B:LEU:HD23 | 16       | 0.11          |
| (1,763)  | 1:212:A:THR:HA   | 1:210:A:LEU:HD11 | 13       | 0.11          |
| (1,763)  | 1:212:A:THR:HA   | 1:210:A:LEU:HD12 | 13       | 0.11          |
| (1,763)  | 1:212:A:THR:HA   | 1:210:A:LEU:HD13 | 13       | 0.11          |
| (1,758)  | 1:206:A:GLN:HG3  | 1:206:A:GLN:HB3  | 4        | 0.11          |
| (1,691)  | 2:654:B:LEU:HD21 | 2:686:B:ARG:H    | 2        | 0.11          |
| (1,691)  | 2:654:B:LEU:HD22 | 2:686:B:ARG:H    | 2        | 0.11          |
| (1,691)  | 2:654:B:LEU:HD23 | 2:686:B:ARG:H    | 2        | 0.11          |
| (1,688)  | 2:696:B:VAL:HG21 | 2:685:B:LEU:H    | 19       | 0.11          |
| (1,688)  | 2:696:B:VAL:HG22 | 2:685:B:LEU:H    | 19       | 0.11          |
| (1,688)  | 2:696:B:VAL:HG23 | 2:685:B:LEU:H    | 19       | 0.11          |
| (1,655)  | 2:672:B:ARG:HG3  | 2:673:B:ILE:H    | 7        | 0.11          |
| (1,625)  | 2:650:B:ALA:HB1  | 2:648:B:GLU:H    | 17       | 0.11          |
| (1,625)  | 2:650:B:ALA:HB2  | 2:648:B:GLU:H    | 17       | 0.11          |
| (1,625)  | 2:650:B:ALA:HB3  | 2:648:B:GLU:H    | 17       | 0.11          |
| (1,624)  | 2:647:B:GLU:HB2  | 2:648:B:GLU:H    | 6        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,614) | 2:640:B:LYS:HB2  | 2:642:B:SER:H    | 3        | 0.11          |
| (1,589) | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 8        | 0.11          |
| (1,589) | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 8        | 0.11          |
| (1,589) | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 8        | 0.11          |
| (1,562) | 2:629:B:ALA:HB1  | 2:632:B:ARG:H    | 3        | 0.11          |
| (1,562) | 2:629:B:ALA:HB2  | 2:632:B:ARG:H    | 3        | 0.11          |
| (1,562) | 2:629:B:ALA:HB3  | 2:632:B:ARG:H    | 3        | 0.11          |
| (1,534) | 2:615:B:ASP:HB2  | 2:615:B:ASP:H    | 10       | 0.11          |
| (1,514) | 2:700:B:LEU:HG   | 2:699:B:ARG:H    | 14       | 0.11          |
| (1,514) | 2:702:B:MET:HE1  | 2:699:B:ARG:H    | 17       | 0.11          |
| (1,514) | 2:702:B:MET:HE2  | 2:699:B:ARG:H    | 17       | 0.11          |
| (1,514) | 2:702:B:MET:HE3  | 2:699:B:ARG:H    | 17       | 0.11          |
| (1,444) | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD21 | 11       | 0.11          |
| (1,444) | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD22 | 11       | 0.11          |
| (1,444) | 2:685:B:LEU:HB3  | 2:658:B:LEU:HD23 | 11       | 0.11          |
| (1,441) | 2:697:B:LEU:HA   | 2:696:B:VAL:HG21 | 4        | 0.11          |
| (1,441) | 2:697:B:LEU:HA   | 2:696:B:VAL:HG22 | 4        | 0.11          |
| (1,441) | 2:697:B:LEU:HA   | 2:696:B:VAL:HG23 | 4        | 0.11          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 13       | 0.11          |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 13       | 0.11          |
| (1,403) | 2:667:B:ARG:HG3  | 2:667:B:ARG:HD2  | 3        | 0.11          |
| (1,396) | 2:632:B:ARG:HG3  | 2:632:B:ARG:HD2  | 12       | 0.11          |
| (1,396) | 2:686:B:ARG:HB2  | 2:686:B:ARG:HD3  | 14       | 0.11          |
| (1,388) | 2:648:B:GLU:HB3  | 2:651:B:LYS:HE2  | 18       | 0.11          |
| (1,315) | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 11       | 0.11          |
| (1,315) | 2:686:B:ARG:HA   | 2:653:B:ARG:HD2  | 14       | 0.11          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB1  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB2  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD21 | 2:669:B:ALA:HB3  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB1  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB2  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD22 | 2:669:B:ALA:HB3  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB1  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB2  | 10       | 0.11          |
| (1,300) | 2:700:B:LEU:HD23 | 2:669:B:ALA:HB3  | 10       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,289)  | 2:631:B:ILE:HG21 | 2:628:B:LEU:HB3  | 20       | 0.11          |
| (1,289)  | 2:631:B:ILE:HG22 | 2:628:B:LEU:HB3  | 20       | 0.11          |
| (1,289)  | 2:631:B:ILE:HG23 | 2:628:B:LEU:HB3  | 20       | 0.11          |
| (1,223)  | 2:716:B:LYS:HG3  | 2:716:B:LYS:HD2  | 3        | 0.11          |
| (1,220)  | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 14       | 0.11          |
| (1,220)  | 2:647:B:GLU:HG2  | 2:647:B:GLU:HB3  | 19       | 0.11          |
| (1,218)  | 2:728:B:LYS:HE3  | 2:728:B:LYS:HD3  | 11       | 0.11          |
| (1,218)  | 2:728:B:LYS:HE3  | 2:728:B:LYS:HD2  | 17       | 0.11          |
| (1,211)  | 2:712:B:ARG:HB2  | 2:712:B:ARG:HG3  | 5        | 0.11          |
| (1,209)  | 2:719:B:ARG:HB3  | 2:719:B:ARG:HG2  | 1        | 0.11          |
| (1,170)  | 2:634:B:LEU:HG   | 2:700:B:LEU:HD21 | 6        | 0.11          |
| (1,170)  | 2:634:B:LEU:HG   | 2:700:B:LEU:HD22 | 6        | 0.11          |
| (1,170)  | 2:634:B:LEU:HG   | 2:700:B:LEU:HD23 | 6        | 0.11          |
| (1,151)  | 2:641:B:LEU:HG   | 2:654:B:LEU:HD11 | 1        | 0.11          |
| (1,151)  | 2:641:B:LEU:HG   | 2:654:B:LEU:HD12 | 1        | 0.11          |
| (1,151)  | 2:641:B:LEU:HG   | 2:654:B:LEU:HD13 | 1        | 0.11          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG21 | 10       | 0.11          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG22 | 10       | 0.11          |
| (1,138)  | 2:634:B:LEU:HB3  | 2:630:B:THR:HG23 | 10       | 0.11          |
| (1,106)  | 2:626:B:THR:HA   | 2:665:B:ILE:HG21 | 20       | 0.11          |
| (1,106)  | 2:626:B:THR:HA   | 2:665:B:ILE:HG22 | 20       | 0.11          |
| (1,106)  | 2:626:B:THR:HA   | 2:665:B:ILE:HG23 | 20       | 0.11          |
| (1,1)    | 2:614:B:GLU:HG2  | 2:614:B:GLU:HB3  | 4        | 0.11          |
| (3,89)   | 2:714:B:PHE:O    | 2:718:B:TRP:H    | 15       | 0.1           |
| (3,4)    | 2:617:B:ARG:O    | 2:621:B:ASP:N    | 6        | 0.1           |
| (3,1)    | 2:616:B:GLU:O    | 2:620:B:LEU:H    | 6        | 0.1           |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB1  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB2  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG21 | 2:692:B:ALA:HB3  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB1  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB2  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG22 | 2:692:B:ALA:HB3  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB1  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB2  | 2        | 0.1           |
| (2,91)   | 1:222:A:THR:HG23 | 2:692:B:ALA:HB3  | 2        | 0.1           |
| (2,2)    | 2:707:B:TRP:HD1  | 2:624:B:LEU:HA   | 5        | 0.1           |
| (1,2749) | 1:221:A:ARG:HG3  | 1:221:A:ARG:H    | 4        | 0.1           |
| (1,2694) | 1:210:A:LEU:HB3  | 1:210:A:LEU:H    | 10       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG21 | 1:217:A:MET:HE1  | 15       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG21 | 1:217:A:MET:HE2  | 15       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG21 | 1:217:A:MET:HE3  | 15       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG22 | 1:217:A:MET:HE1  | 15       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2668) | 1:216:A:ILE:HG22 | 1:217:A:MET:HE2  | 15       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG22 | 1:217:A:MET:HE3  | 15       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG23 | 1:217:A:MET:HE1  | 15       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG23 | 1:217:A:MET:HE2  | 15       | 0.1           |
| (1,2668) | 1:216:A:ILE:HG23 | 1:217:A:MET:HE3  | 15       | 0.1           |
| (1,2659) | 1:223:A:LEU:HA   | 1:226:A:LEU:HB2  | 2        | 0.1           |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD21 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD22 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG21 | 1:223:A:LEU:HD23 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD21 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD22 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG22 | 1:223:A:LEU:HD23 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD21 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD22 | 14       | 0.1           |
| (1,2640) | 2:681:B:ILE:HG23 | 1:223:A:LEU:HD23 | 14       | 0.1           |
| (1,2613) | 1:221:A:ARG:HB2  | 1:221:A:ARG:HG3  | 7        | 0.1           |
| (1,2610) | 2:680:B:ASP:HB3  | 1:220:A:LEU:HD21 | 16       | 0.1           |
| (1,2610) | 2:680:B:ASP:HB3  | 1:220:A:LEU:HD22 | 16       | 0.1           |
| (1,2610) | 2:680:B:ASP:HB3  | 1:220:A:LEU:HD23 | 16       | 0.1           |
| (1,2609) | 2:680:B:ASP:HA   | 1:220:A:LEU:HD21 | 17       | 0.1           |
| (1,2609) | 2:680:B:ASP:HA   | 1:220:A:LEU:HD22 | 17       | 0.1           |
| (1,2609) | 2:680:B:ASP:HA   | 1:220:A:LEU:HD23 | 17       | 0.1           |
| (1,2604) | 2:681:B:ILE:HA   | 1:220:A:LEU:HD11 | 20       | 0.1           |
| (1,2604) | 2:681:B:ILE:HA   | 1:220:A:LEU:HD12 | 20       | 0.1           |
| (1,2604) | 2:681:B:ILE:HA   | 1:220:A:LEU:HD13 | 20       | 0.1           |
| (1,2489) | 2:707:B:TRP:HA   | 1:207:A:LEU:HD21 | 15       | 0.1           |
| (1,2489) | 2:707:B:TRP:HA   | 1:207:A:LEU:HD22 | 15       | 0.1           |
| (1,2489) | 2:707:B:TRP:HA   | 1:207:A:LEU:HD23 | 15       | 0.1           |
| (1,2278) | 2:689:B:PRO:HG2  | 2:688:B:ASN:H    | 19       | 0.1           |
| (1,2239) | 2:687:B:LYS:HE2  | 2:684:B:GLY:H    | 10       | 0.1           |
| (1,2132) | 2:728:B:LYS:HG3  | 2:728:B:LYS:H    | 4        | 0.1           |
| (1,2046) | 2:643:B:ARG:HG2  | 2:643:B:ARG:H    | 11       | 0.1           |
| (1,1863) | 2:696:B:VAL:HB   | 2:697:B:LEU:H    | 1        | 0.1           |
| (1,1706) | 2:681:B:ILE:HG21 | 2:670:B:LEU:HD21 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG21 | 2:670:B:LEU:HD22 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG21 | 2:670:B:LEU:HD23 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG22 | 2:670:B:LEU:HD21 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG22 | 2:670:B:LEU:HD22 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG22 | 2:670:B:LEU:HD23 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG23 | 2:670:B:LEU:HD21 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG23 | 2:670:B:LEU:HD22 | 11       | 0.1           |
| (1,1706) | 2:681:B:ILE:HG23 | 2:670:B:LEU:HD23 | 11       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1645) | 1:220:A:LEU:HD21 | 2:677:B:LYS:HE3  | 4        | 0.1           |
| (1,1645) | 1:220:A:LEU:HD22 | 2:677:B:LYS:HE3  | 4        | 0.1           |
| (1,1645) | 1:220:A:LEU:HD23 | 2:677:B:LYS:HE3  | 4        | 0.1           |
| (1,1561) | 2:716:B:LYS:HD2  | 2:716:B:LYS:HA   | 5        | 0.1           |
| (1,1539) | 2:702:B:MET:HB3  | 2:699:B:ARG:HA   | 1        | 0.1           |
| (1,1312) | 2:698:B:LYS:HB3  | 2:698:B:LYS:HD3  | 7        | 0.1           |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD21 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD22 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG11 | 2:700:B:LEU:HD23 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD21 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD22 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG12 | 2:700:B:LEU:HD23 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD21 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD22 | 12       | 0.1           |
| (1,1251) | 2:633:B:VAL:HG13 | 2:700:B:LEU:HD23 | 12       | 0.1           |
| (1,1241) | 2:681:B:ILE:HD11 | 2:670:B:LEU:HD11 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD11 | 2:670:B:LEU:HD12 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD11 | 2:670:B:LEU:HD13 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD12 | 2:670:B:LEU:HD11 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD12 | 2:670:B:LEU:HD12 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD12 | 2:670:B:LEU:HD13 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD13 | 2:670:B:LEU:HD11 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD13 | 2:670:B:LEU:HD12 | 8        | 0.1           |
| (1,1241) | 2:681:B:ILE:HD13 | 2:670:B:LEU:HD13 | 8        | 0.1           |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD11 | 8        | 0.1           |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD12 | 8        | 0.1           |
| (1,1194) | 2:670:B:LEU:HB3  | 2:682:B:ILE:HD13 | 8        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD21 | 3        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD22 | 3        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD23 | 3        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD21 | 6        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD22 | 6        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD23 | 6        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD21 | 8        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD22 | 8        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD23 | 8        | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD21 | 11       | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD22 | 11       | 0.1           |
| (1,1170) | 2:670:B:LEU:HB2  | 2:670:B:LEU:HD23 | 11       | 0.1           |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD11 | 3        | 0.1           |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD12 | 3        | 0.1           |
| (1,1154) | 2:654:B:LEU:HB3  | 2:654:B:LEU:HD13 | 3        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG11 | 6        | 0.1           |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG12 | 6        | 0.1           |
| (1,883) | 2:661:B:THR:HA   | 2:664:B:VAL:HG13 | 6        | 0.1           |
| (1,758) | 1:214:A:GLU:HG2  | 1:214:A:GLU:HB3  | 7        | 0.1           |
| (1,758) | 1:206:A:GLN:HG2  | 1:206:A:GLN:HB3  | 12       | 0.1           |
| (1,670) | 2:674:B:TYR:HB3  | 2:678:B:ALA:H    | 19       | 0.1           |
| (1,624) | 2:647:B:GLU:HB2  | 2:648:B:GLU:H    | 1        | 0.1           |
| (1,558) | 2:634:B:LEU:HD21 | 2:634:B:LEU:H    | 13       | 0.1           |
| (1,558) | 2:634:B:LEU:HD22 | 2:634:B:LEU:H    | 13       | 0.1           |
| (1,558) | 2:634:B:LEU:HD23 | 2:634:B:LEU:H    | 13       | 0.1           |
| (1,521) | 2:675:B:ALA:HB1  | 2:677:B:LYS:H    | 13       | 0.1           |
| (1,521) | 2:675:B:ALA:HB2  | 2:677:B:LYS:H    | 13       | 0.1           |
| (1,521) | 2:675:B:ALA:HB3  | 2:677:B:LYS:H    | 13       | 0.1           |
| (1,463) | 2:645:B:SER:HB2  | 2:649:B:GLN:HE22 | 10       | 0.1           |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD11 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD12 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG21 | 2:670:B:LEU:HD13 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD11 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD12 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG22 | 2:670:B:LEU:HD13 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD11 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD12 | 2        | 0.1           |
| (1,434) | 2:630:B:THR:HG23 | 2:670:B:LEU:HD13 | 2        | 0.1           |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD11 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD12 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB1  | 2:691:B:ILE:HD13 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD11 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD12 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB2  | 2:691:B:ILE:HD13 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD11 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD12 | 15       | 0.1           |
| (1,422) | 2:692:B:ALA:HB3  | 2:691:B:ILE:HD13 | 15       | 0.1           |
| (1,366) | 2:671:B:GLN:HB2  | 2:668:B:LYS:HA   | 5        | 0.1           |
| (1,297) | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB1  | 4        | 0.1           |
| (1,297) | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB2  | 4        | 0.1           |
| (1,297) | 2:665:B:ILE:HG12 | 2:629:B:ALA:HB3  | 4        | 0.1           |
| (1,250) | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB1  | 9        | 0.1           |
| (1,250) | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB2  | 9        | 0.1           |
| (1,250) | 2:649:B:GLN:HB2  | 2:646:B:ALA:HB3  | 9        | 0.1           |
| (1,237) | 2:613:B:CYS:HB3  | 2:614:B:GLU:HG2  | 20       | 0.1           |
| (1,218) | 2:698:B:LYS:HE2  | 2:698:B:LYS:HD3  | 1        | 0.1           |
| (1,214) | 2:640:B:LYS:HG3  | 2:637:B:ILE:HG13 | 17       | 0.1           |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,122) | 2:672:B:ARG:HG2 | 2:623:B:VAL:HG21 | 5        | 0.1           |
| (1,122) | 2:672:B:ARG:HG2 | 2:623:B:VAL:HG22 | 5        | 0.1           |
| (1,122) | 2:672:B:ARG:HG2 | 2:623:B:VAL:HG23 | 5        | 0.1           |
| (1,71)  | 2:723:B:GLU:HA  | 2:723:B:GLU:HB3  | 11       | 0.1           |

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

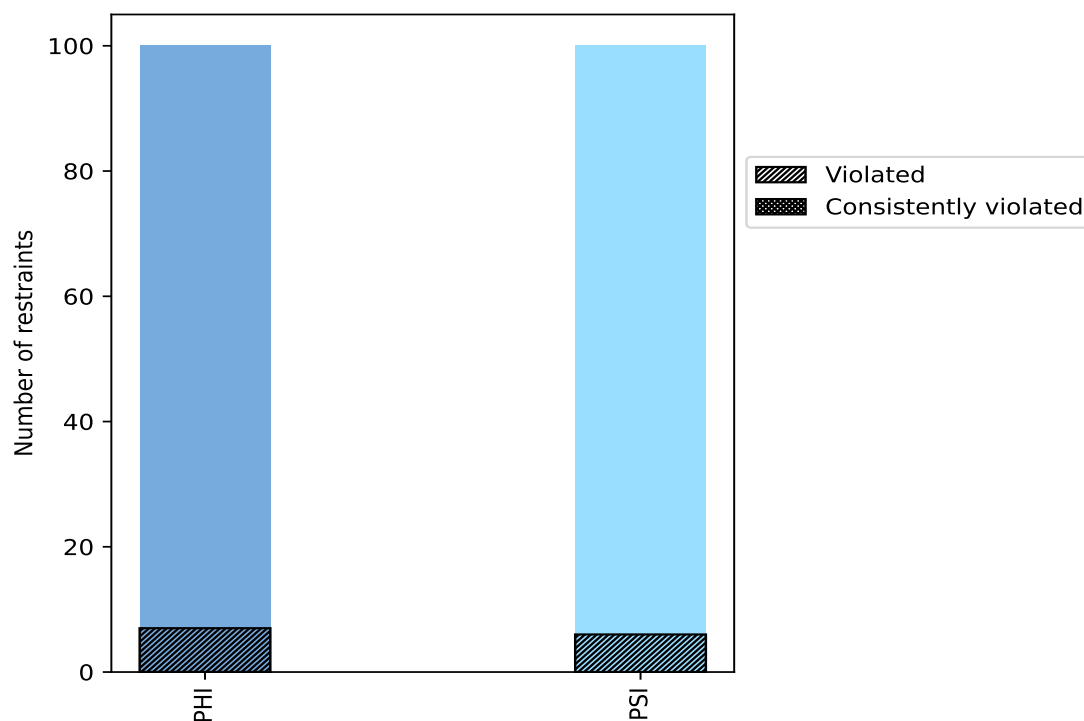
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PHI        | 100   | 50.0           | 7                     | 7.0            | 3.5            | 0                                  | 0.0            | 0.0            |
| PSI        | 100   | 50.0           | 6                     | 6.0            | 3.0            | 0                                  | 0.0            | 0.0            |
| Total      | 200   | 100.0          | 13                    | 6.5            | 6.5            | 0                                  | 0.0            | 0.0            |

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

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



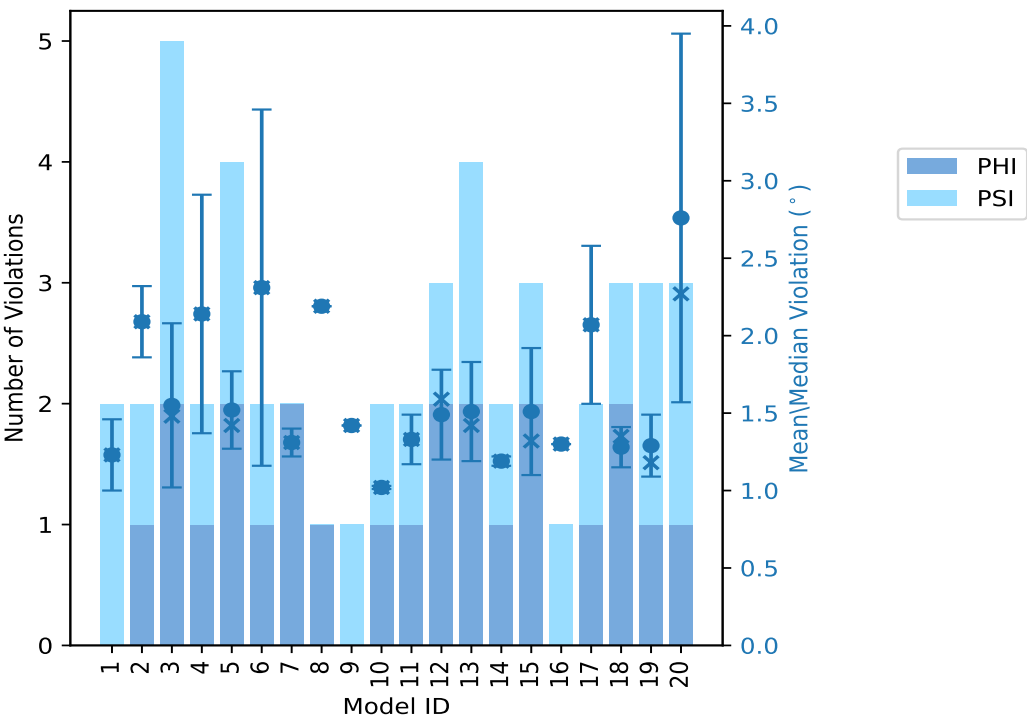
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 0                    | 2   | 2     | 1.23     | 1.46    | 0.23   | 1.23       |
| 2        | 1                    | 1   | 2     | 2.09     | 2.32    | 0.23   | 2.09       |
| 3        | 2                    | 3   | 5     | 1.55     | 2.52    | 0.53   | 1.48       |
| 4        | 1                    | 1   | 2     | 2.14     | 2.92    | 0.77   | 2.14       |
| 5        | 2                    | 2   | 4     | 1.52     | 1.94    | 0.25   | 1.42       |
| 6        | 1                    | 1   | 2     | 2.31     | 3.46    | 1.15   | 2.31       |
| 7        | 2                    | 0   | 2     | 1.31     | 1.4     | 0.09   | 1.31       |
| 8        | 1                    | 0   | 1     | 2.19     | 2.19    | 0.0    | 2.19       |
| 9        | 0                    | 1   | 1     | 1.42     | 1.42    | 0.0    | 1.42       |
| 10       | 1                    | 1   | 2     | 1.02     | 1.02    | 0.01   | 1.02       |
| 11       | 1                    | 1   | 2     | 1.33     | 1.49    | 0.16   | 1.33       |
| 12       | 2                    | 1   | 3     | 1.49     | 1.78    | 0.29   | 1.59       |
| 13       | 2                    | 2   | 4     | 1.51     | 2.03    | 0.32   | 1.42       |
| 14       | 1                    | 1   | 2     | 1.19     | 1.22    | 0.03   | 1.19       |
| 15       | 2                    | 1   | 3     | 1.51     | 2.08    | 0.41   | 1.32       |
| 16       | 0                    | 1   | 1     | 1.3      | 1.3     | 0.0    | 1.3        |
| 17       | 1                    | 1   | 2     | 2.07     | 2.58    | 0.51   | 2.07       |
| 18       | 2                    | 1   | 3     | 1.28     | 1.38    | 0.13   | 1.35       |
| 19       | 1                    | 2   | 3     | 1.29     | 1.57    | 0.2    | 1.18       |
| 20       | 1                    | 2   | 3     | 2.76     | 4.4     | 1.19   | 2.27       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

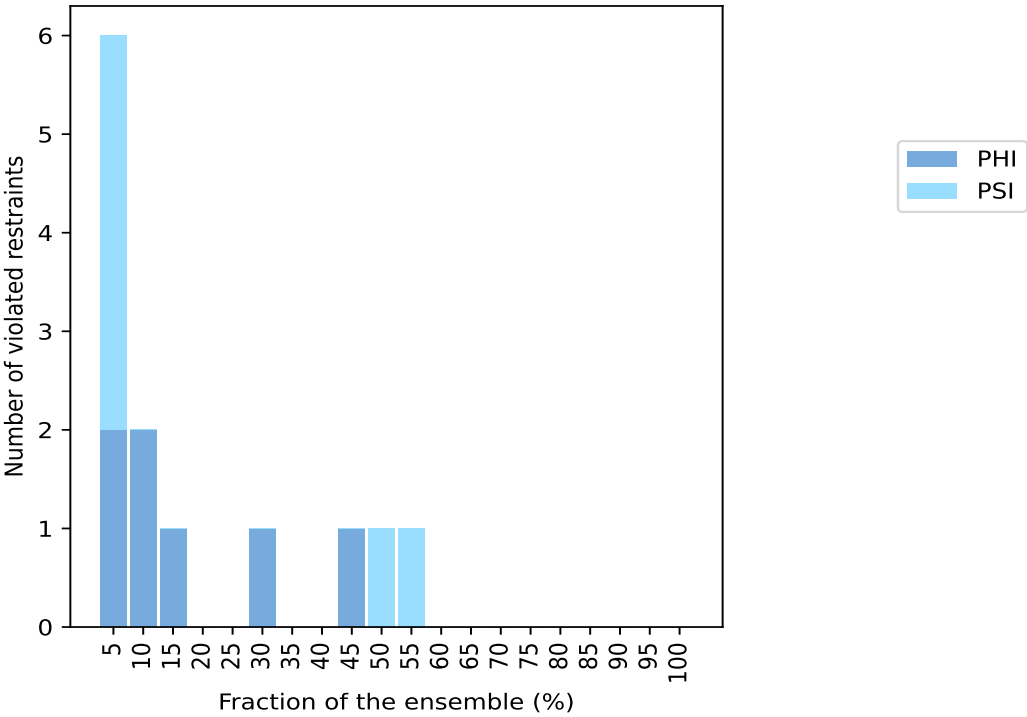
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |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

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

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

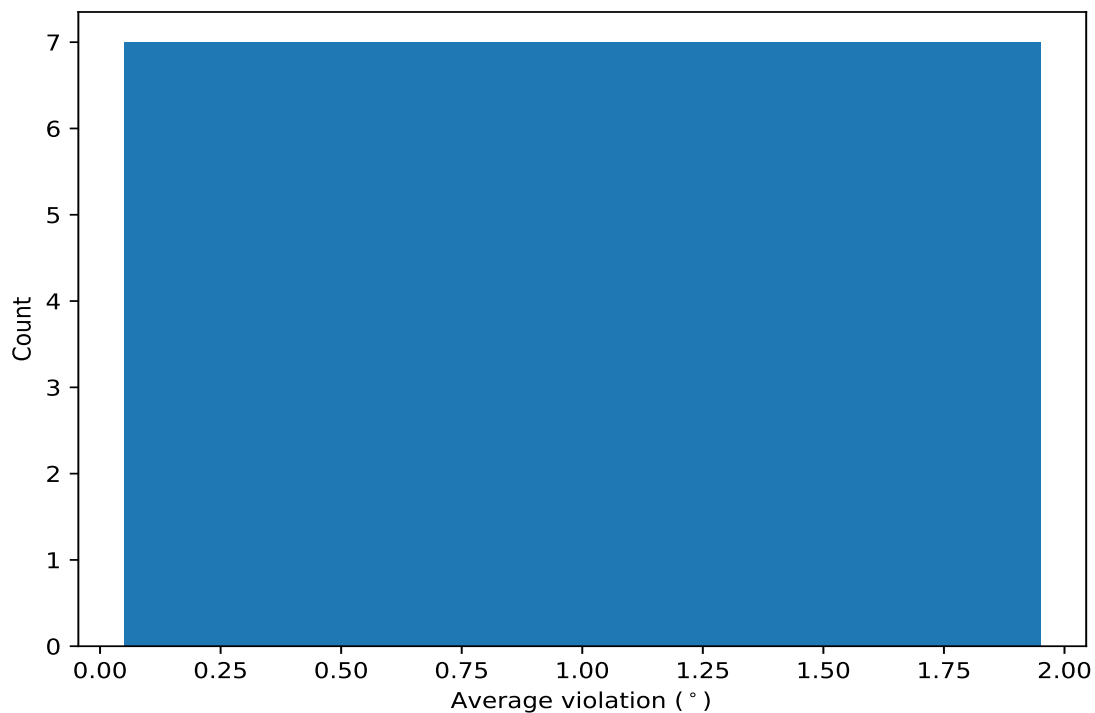


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

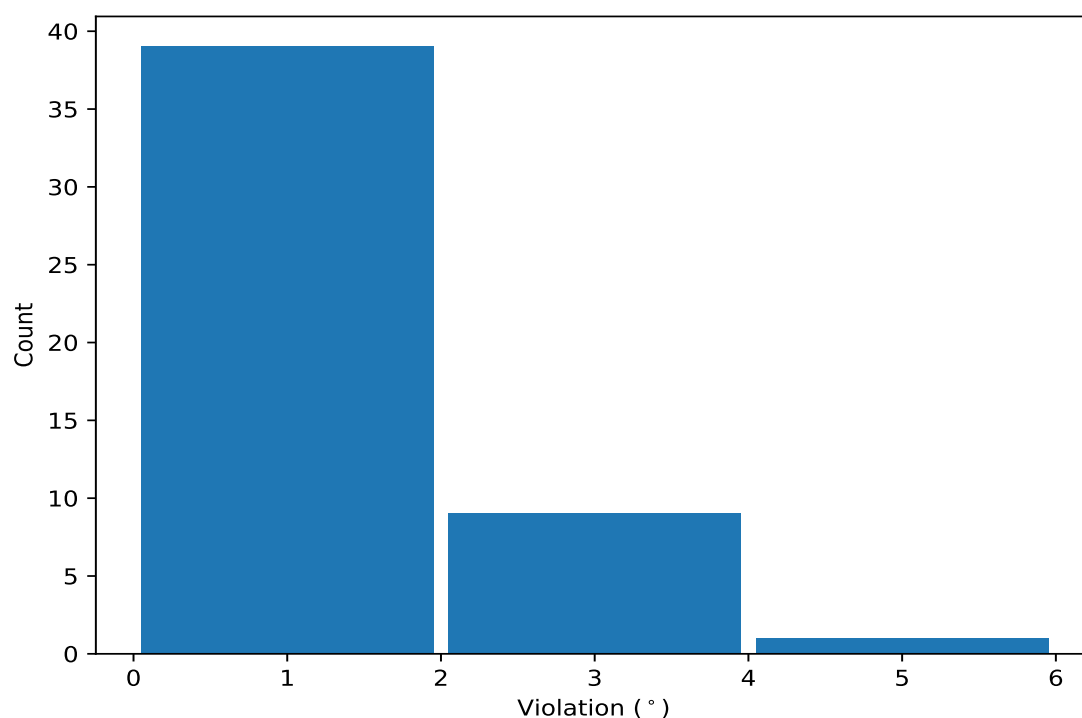
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 11                  | 1.89 | 0.73            | 1.62   |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 10                  | 1.36 | 0.16            | 1.34   |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 9                   | 1.71 | 0.58            | 1.78   |
| (1,86)  | 2:721:B:GLN:C | 2:722:B:ASN:N  | 2:722:B:ASN:CA | 2:722:B:ASN:C | 6                   | 1.45 | 0.38            | 1.34   |
| (1,85)  | 2:720:B:GLU:C | 2:721:B:GLN:N  | 2:721:B:GLN:CA | 2:721:B:GLN:C | 3                   | 1.18 | 0.11            | 1.1    |
| (1,42)  | 2:674:B:TYR:C | 2:675:B:ALA:N  | 2:675:B:ALA:CA | 2:675:B:ALA:C | 2                   | 1.65 | 0.43            | 1.65   |
| (1,87)  | 2:722:B:ASN:C | 2:723:B:GLU:N  | 2:723:B:GLU:CA | 2:723:B:GLU:C | 2                   | 1.31 | 0.26            | 1.31   |

<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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,200) | 1:225:A:LYS:N | 1:225:A:LYS:CA | 1:225:A:LYS:C  | 1:226:A:LEU:N | 20       | 4.4           |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 6        | 3.46          |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 4        | 2.92          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 17       | 2.58          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 3        | 2.52          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 2        | 2.32          |
| (1,86)  | 2:721:B:GLN:C | 2:722:B:ASN:N  | 2:722:B:ASN:CA | 2:722:B:ASN:C | 20       | 2.27          |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 8        | 2.19          |
| (1,42)  | 2:674:B:TYR:C | 2:675:B:ALA:N  | 2:675:B:ALA:CA | 2:675:B:ALA:C | 15       | 2.08          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 13       | 2.03          |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 5        | 1.94          |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 2        | 1.86          |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 12       | 1.78          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 20       | 1.62          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 3        | 1.61          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 12       | 1.59          |
| (1,139) | 2:686:B:ARG:N | 2:686:B:ARG:CA | 2:686:B:ARG:C  | 2:687:B:LYS:N | 19       | 1.57          |
| (1,87)  | 2:722:B:ASN:C | 2:723:B:GLU:N  | 2:723:B:GLU:CA | 2:723:B:GLU:C | 17       | 1.56          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 5        | 1.5           |
| (1,27)  | 2:644:B:LEU:C | 2:645:B:SER:N  | 2:645:B:SER:CA | 2:645:B:SER:C | 11       | 1.49          |
| (1,174) | 2:723:B:GLU:N | 2:723:B:GLU:CA | 2:723:B:GLU:C  | 2:724:B:LYS:N | 3        | 1.48          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 1        | 1.46          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 13       | 1.43          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 9        | 1.42          |
| (1,86)  | 2:721:B:GLN:C | 2:722:B:ASN:N  | 2:722:B:ASN:CA | 2:722:B:ASN:C | 7        | 1.4           |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 13       | 1.4           |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 18       | 1.38          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 4        | 1.37          |
| (1,86)  | 2:721:B:GLN:C | 2:722:B:ASN:N  | 2:722:B:ASN:CA | 2:722:B:ASN:C | 18       | 1.35          |
| (1,85)  | 2:720:B:GLU:C | 2:721:B:GLN:N  | 2:721:B:GLN:CA | 2:721:B:GLN:C | 5        | 1.33          |
| (1,86)  | 2:721:B:GLN:C | 2:722:B:ASN:N  | 2:722:B:ASN:CA | 2:722:B:ASN:C | 15       | 1.32          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 5        | 1.31          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 16       | 1.3           |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 14       | 1.22          |
| (1,42)  | 2:674:B:TYR:C | 2:675:B:ALA:N  | 2:675:B:ALA:CA | 2:675:B:ALA:C | 7        | 1.22          |
| (1,86)  | 2:721:B:GLN:C | 2:722:B:ASN:N  | 2:722:B:ASN:CA | 2:722:B:ASN:C | 13       | 1.18          |
| (1,86)  | 2:721:B:GLN:C | 2:722:B:ASN:N  | 2:722:B:ASN:CA | 2:722:B:ASN:C | 19       | 1.18          |
| (1,113) | 2:641:B:LEU:N | 2:641:B:LEU:CA | 2:641:B:LEU:C  | 2:642:B:SER:N | 11       | 1.17          |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 6        | 1.16          |
| (1,1)   | 2:615:B:ASP:C | 2:616:B:GLU:N  | 2:616:B:GLU:CA | 2:616:B:GLU:C | 14       | 1.16          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 15       | 1.14          |
| (1,127) | 2:671:B:GLN:N | 2:671:B:GLN:CA | 2:671:B:GLN:C  | 2:672:B:ARG:N | 19       | 1.13          |
| (1,85)  | 2:720:B:GLU:C | 2:721:B:GLN:N  | 2:721:B:GLN:CA | 2:721:B:GLN:C | 3        | 1.1           |
| (1,85)  | 2:720:B:GLU:C | 2:721:B:GLN:N  | 2:721:B:GLN:CA | 2:721:B:GLN:C | 12       | 1.1           |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 18       | 1.1           |
| (1,87)  | 2:722:B:ASN:C | 2:723:B:GLU:N  | 2:723:B:GLU:CA | 2:723:B:GLU:C | 3        | 1.05          |
| (1,78)  | 2:713:B:GLY:C | 2:714:B:PHE:N  | 2:714:B:PHE:CA | 2:714:B:PHE:C | 10       | 1.02          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 10       | 1.01          |
| (1,165) | 2:714:B:PHE:N | 2:714:B:PHE:CA | 2:714:B:PHE:C  | 2:715:B:ASN:N | 1        | 1.0           |