



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 12:12 PM UTC

PDB ID : 8E1D / pdb\_00008e1d  
BMRB ID : 31038  
Title : NMR-derived ensemble of the TAZ2 domain of p300 bound to the microphth  
almia-associated transcription factor  
Authors : Langelaan, D.N.; Branch, M.  
Deposited on : 2022-08-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

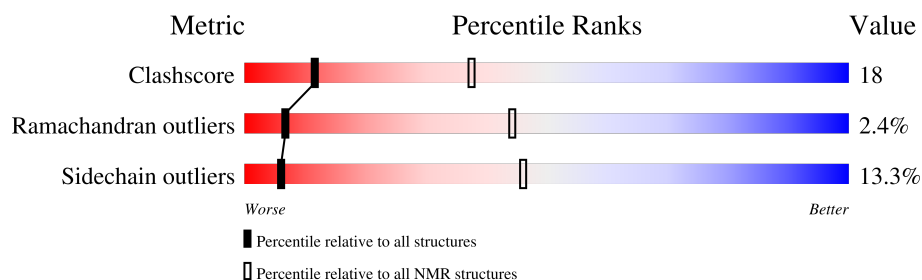
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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



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

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

| Mol | Chain | Length | Quality of chain                                           |
|-----|-------|--------|------------------------------------------------------------|
| 1   | B     | 34     | <div> <div>18%</div> <div>9%</div> <div>74%</div> </div>   |
| 2   | A     | 92     | <div> <div>63%</div> <div>26%</div> <div>• 8%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                        |                   |              |
|--------------------------------------|----------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                  | Backbone RMSD (Å) | Medoid model |
| 1                                    | B:126-B:134,<br>A:1727-<br>A:1811 (94) | 0.91              | 4            |

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

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

The models can be grouped into 3 clusters and 6 single-model clusters were found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1922 atoms, of which 964 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Microphthalmia-associated transcription factor.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | B     | 34       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 498   | 154 | 242 | 39 | 59 | 4 |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 108     | GLY      | -      | expression tag | UNP O75030 |

- Molecule 2 is a protein called Histone acetyltransferase p300.

| Mol | Chain | Residues | Atoms |     |     |     |     |    | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|-------|
| 2   | A     | 92       | Total | C   | H   | N   | O   | S  | 0     |
|     |       |          | 1421  | 425 | 722 | 142 | 122 | 10 |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 1721    | GLY      | -      | expression tag      | UNP Q09472 |
| A     | 1722    | SER      | -      | expression tag      | UNP Q09472 |
| A     | 1738    | ALA      | CYS    | engineered mutation | UNP Q09472 |
| A     | 1746    | ALA      | CYS    | engineered mutation | UNP Q09472 |
| A     | 1789    | ALA      | CYS    | engineered mutation | UNP Q09472 |
| A     | 1790    | ALA      | CYS    | engineered mutation | UNP Q09472 |

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

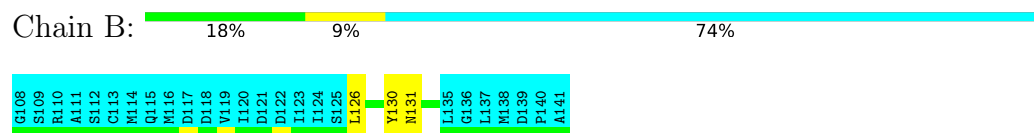
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 3   | A     | 3        | Total | Zn |
|     |       |          | 3     | 3  |

## 4 Residue-property plots

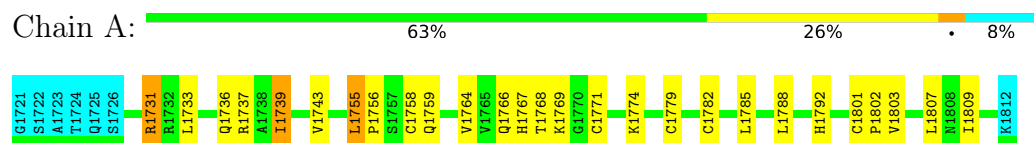
### 4.1 Average score per residue in the NMR ensemble

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: Microphthalmia-associated transcription factor



- Molecule 2: Histone acetyltransferase p300

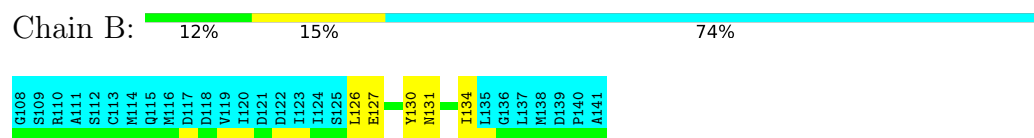


### 4.2 Scores per residue for each member of the ensemble

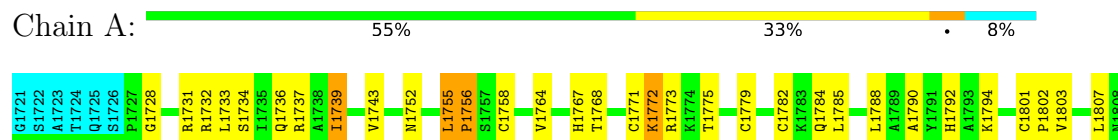
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Microphthalmia-associated transcription factor



- Molecule 2: Histone acetyltransferase p300





#### 4.2.2 Score per residue for model 2

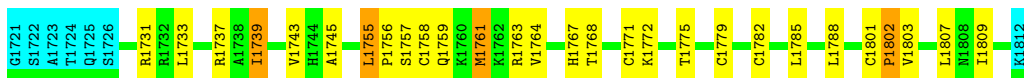
- Molecule 1: Microphthalmia-associated transcription factor

Chain B: 15% 9% 74%



- Molecule 2: Histone acetyltransferase p300

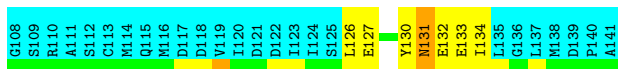
Chain A: 62% 26% 8%



#### 4.2.3 Score per residue for model 3

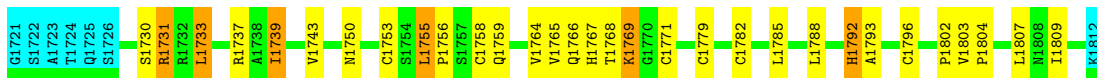
- Molecule 1: Microphthalmia-associated transcription factor

Chain B: 6% 18% 74%



- Molecule 2: Histone acetyltransferase p300

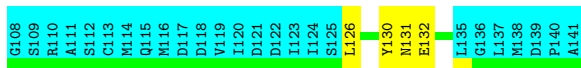
Chain A: 59% 27% 7% 8%



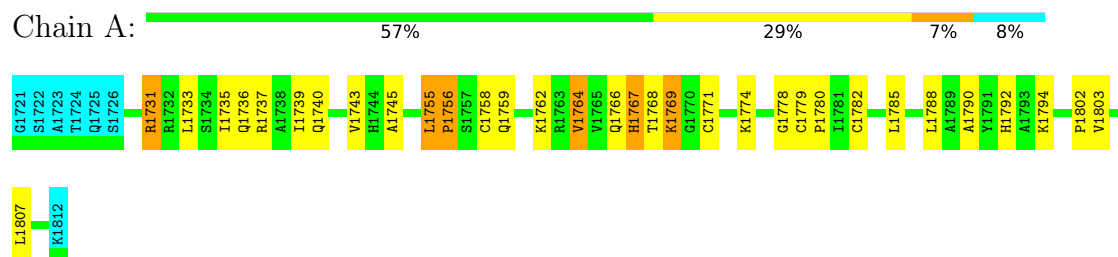
#### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Microphthalmia-associated transcription factor

Chain B: 15% 12% 74%

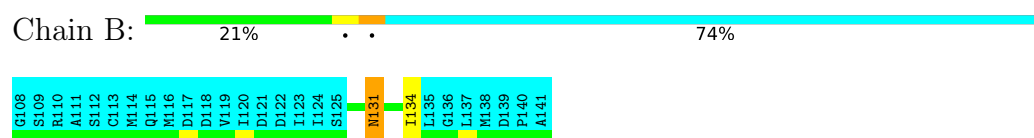


- Molecule 2: Histone acetyltransferase p300

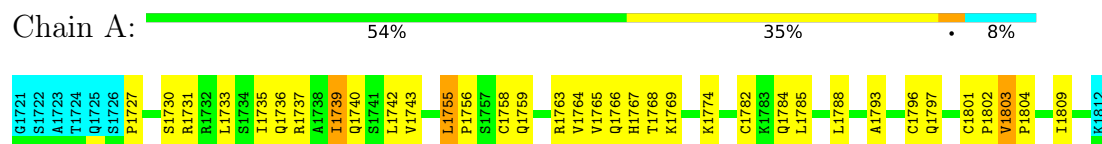


#### 4.2.5 Score per residue for model 5

- Molecule 1: Microphthalmia-associated transcription factor

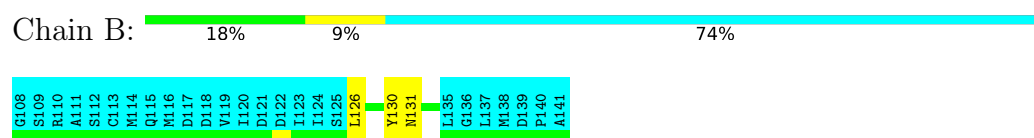


- Molecule 2: Histone acetyltransferase p300

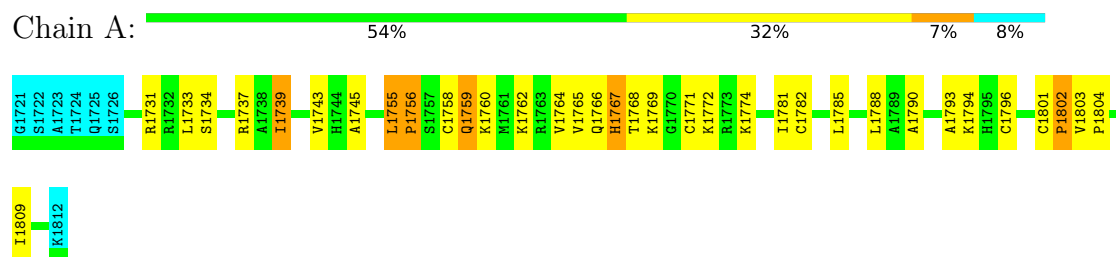


#### 4.2.6 Score per residue for model 6

- Molecule 1: Microphthalmia-associated transcription factor

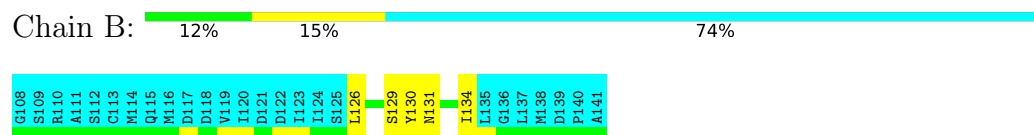


- Molecule 2: Histone acetyltransferase p300

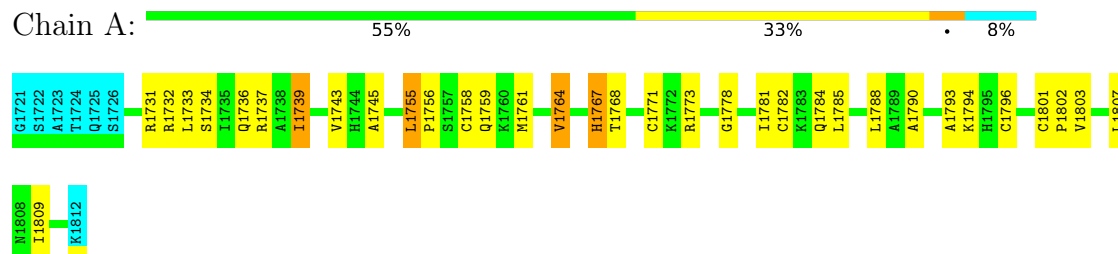


### 4.2.7 Score per residue for model 7

- Molecule 1: Microphthalmia-associated transcription factor

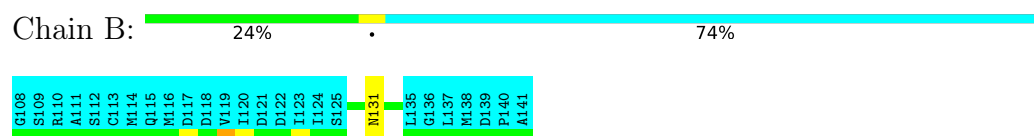


- Molecule 2: Histone acetyltransferase p300

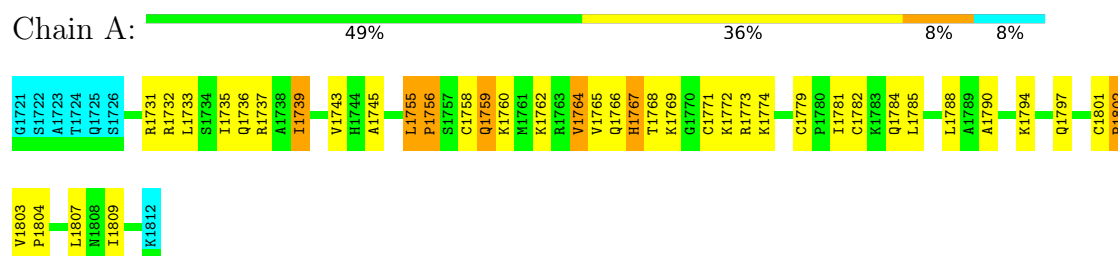


### 4.2.8 Score per residue for model 8

- Molecule 1: Microphthalmia-associated transcription factor

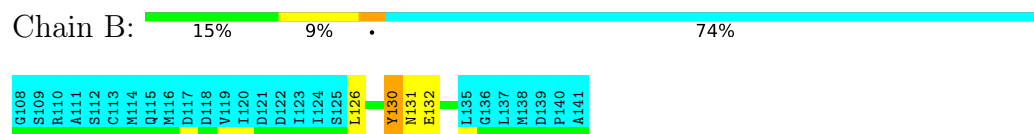


- Molecule 2: Histone acetyltransferase p300

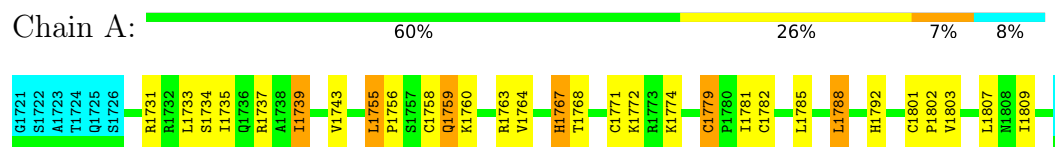


### 4.2.9 Score per residue for model 9

- Molecule 1: Microphthalmia-associated transcription factor

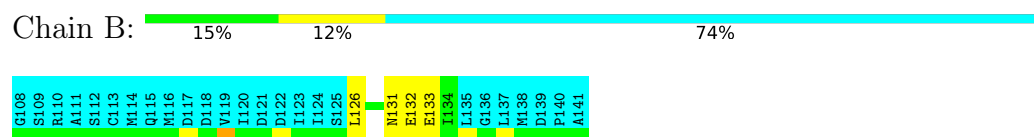


- Molecule 2: Histone acetyltransferase p300

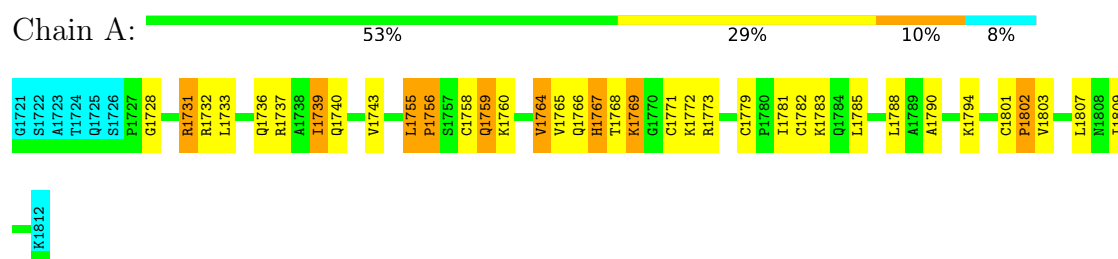


#### 4.2.10 Score per residue for model 10

- Molecule 1: Microphthalmia-associated transcription factor

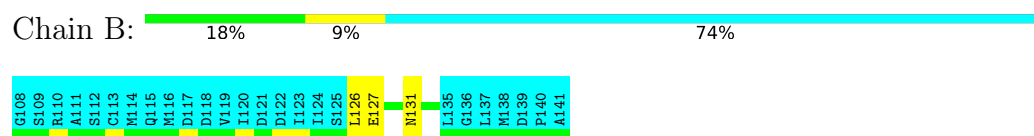


- Molecule 2: Histone acetyltransferase p300

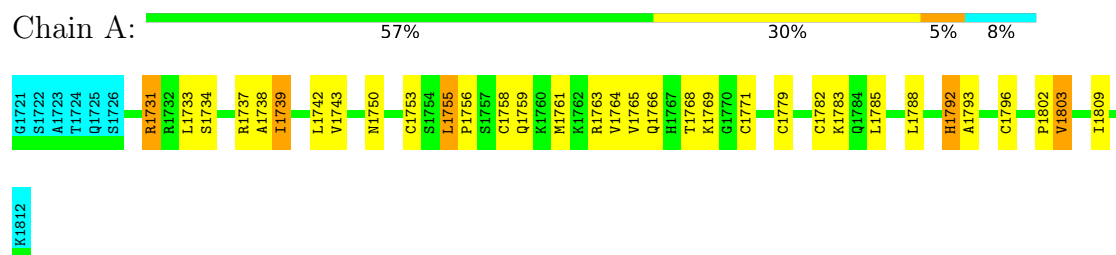


#### 4.2.11 Score per residue for model 11

- Molecule 1: Microphthalmia-associated transcription factor

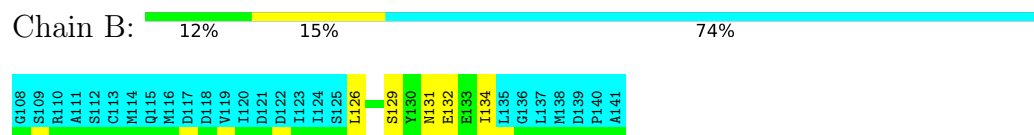


- Molecule 2: Histone acetyltransferase p300

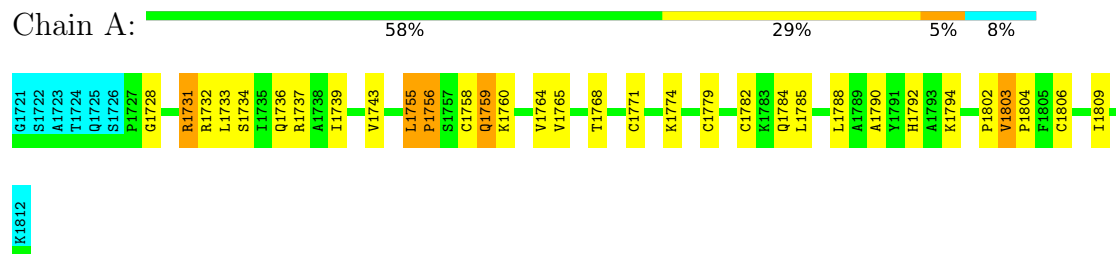


### 4.2.12 Score per residue for model 12

- Molecule 1: Microphthalmia-associated transcription factor

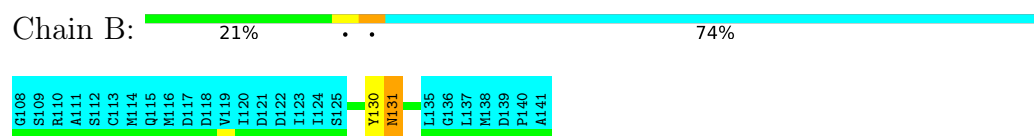


- Molecule 2: Histone acetyltransferase p300

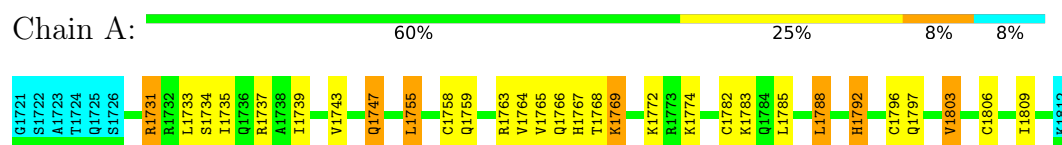


### 4.2.13 Score per residue for model 13

- Molecule 1: Microphthalmia-associated transcription factor

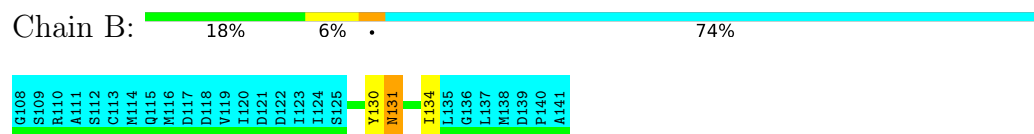


- Molecule 2: Histone acetyltransferase p300



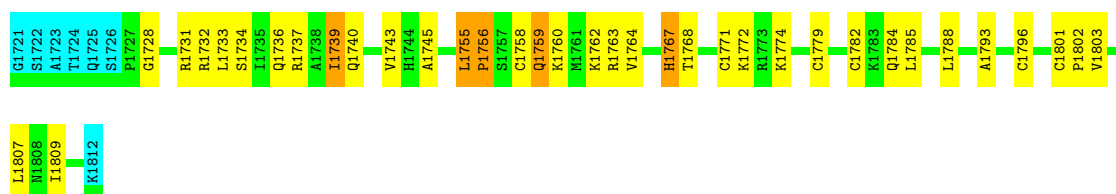
### 4.2.14 Score per residue for model 14

- Molecule 1: Microphthalmia-associated transcription factor



- Molecule 2: Histone acetyltransferase p300





#### 4.2.15 Score per residue for model 15

- Molecule 1: Microphthalmia-associated transcription factor

Chain B: 18% 6% . 74%



- Molecule 2: Histone acetyltransferase p300

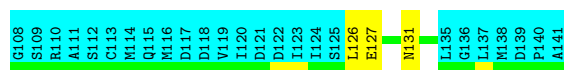
Chain A: 58% 28% 7% 8%



#### 4.2.16 Score per residue for model 16

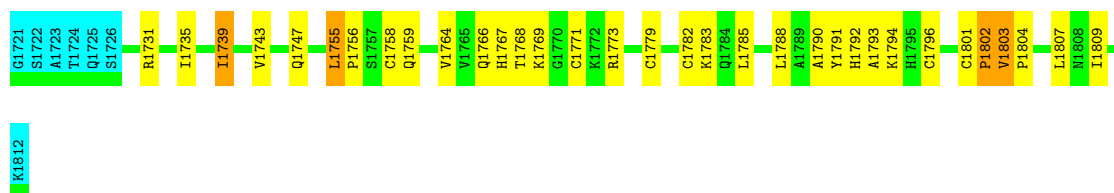
- Molecule 1: Microphthalmia-associated transcription factor

Chain B: 18% 9% 74%



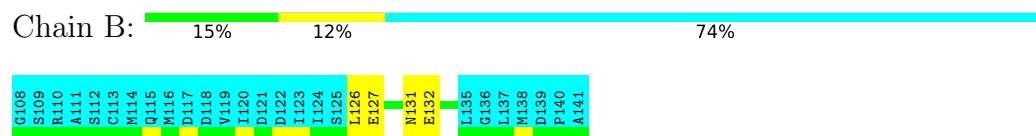
- Molecule 2: Histone acetyltransferase p300

Chain A: 57% 32% . 8%

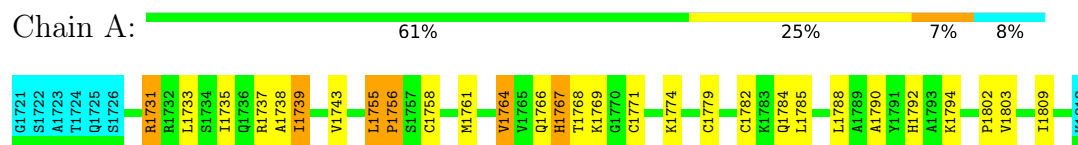


#### 4.2.17 Score per residue for model 17

- Molecule 1: Microphthalmia-associated transcription factor

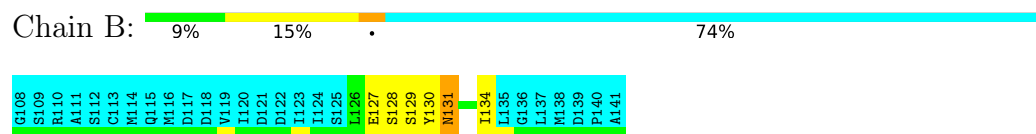


- Molecule 2: Histone acetyltransferase p300

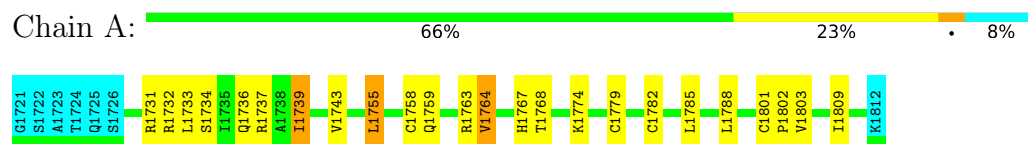


#### 4.2.18 Score per residue for model 18

- Molecule 1: Microphthalmia-associated transcription factor

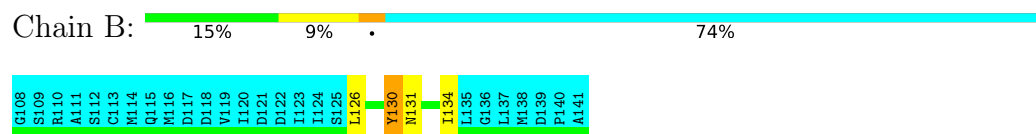


- Molecule 2: Histone acetyltransferase p300

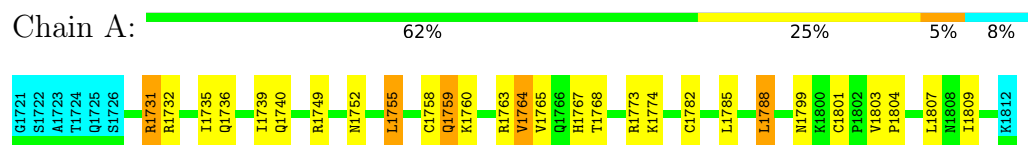


#### 4.2.19 Score per residue for model 19

- Molecule 1: Microphthalmia-associated transcription factor

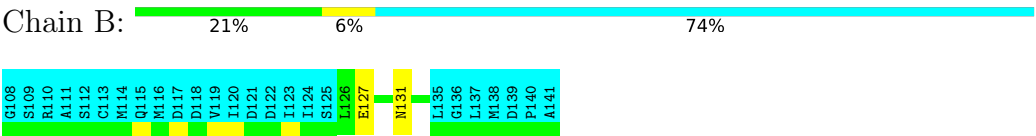


- Molecule 2: Histone acetyltransferase p300

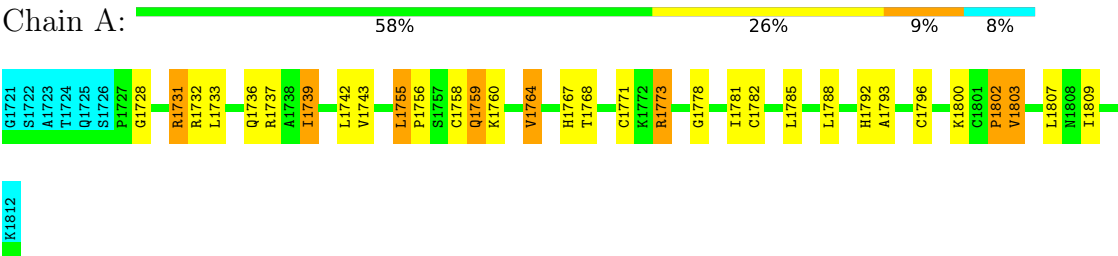


4.2.20 Score per residue for model 20

- Molecule 1: Microphthalmia-associated transcription factor



- Molecule 2: Histone acetyltransferase p300



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | refinement            |         |
| CNS           | refinement            |         |
| ARIA          | structure calculation |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1435           |
| Number of shifts mapped to atoms             | 1435           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 87%            |

## 6 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | B     | 0.40±0.04    | 0±0/76 ( 0.0± 0.0%)  | 0.70±0.06   | 0±0/103 ( 0.0± 0.0%) |
| 2   | A     | 0.51±0.01    | 0±0/663 ( 0.0± 0.0%) | 0.89±0.02   | 0±0/889 ( 0.0± 0.0%) |
| All | All   | 0.50         | 0/14780 ( 0.0%)      | 0.87        | 2/19840 ( 0.0%)      |

There are no bond-length outliers.

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

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|------|------|--------|------|-------------|----------|--------|-------|
|     |       |      |      |        |      |             |          | Worst  | Total |
| 2   | A     | 1803 | VAL  | CA-C-N | 5.17 | 124.48      | 118.85   | 16     | 1     |
| 2   | A     | 1803 | VAL  | C-N-CA | 5.17 | 124.48      | 118.85   | 16     | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | B     | 75    | 65       | 65       | 2±1     |
| 2   | A     | 652   | 674      | 673      | 25±4    |
| All | All   | 14600 | 14780    | 14760    | 520     |

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 18.

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

| Atom-1            | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-------------------|-------------------|----------|-------------|--------|-------|
|                   |                   |          |             | Worst  | Total |
| 2:A:1782:CYS:HA   | 2:A:1785:LEU:HD12 | 0.80     | 1.54        | 19     | 11    |
| 2:A:1768:THR:HG21 | 2:A:1785:LEU:HD22 | 0.79     | 1.53        | 18     | 9     |
| 2:A:1768:THR:HA   | 2:A:1771:CYS:SG   | 0.78     | 2.19        | 3      | 11    |
| 2:A:1755:LEU:CD1  | 2:A:1758:CYS:HB3  | 0.78     | 2.09        | 17     | 8     |
| 2:A:1755:LEU:HD11 | 2:A:1758:CYS:HB3  | 0.77     | 1.56        | 8      | 8     |
| 2:A:1793:ALA:HA   | 2:A:1796:CYS:SG   | 0.76     | 2.20        | 3      | 9     |
| 2:A:1755:LEU:HD21 | 2:A:1758:CYS:H    | 0.73     | 1.44        | 10     | 8     |
| 2:A:1755:LEU:C    | 2:A:1755:LEU:HD13 | 0.71     | 2.09        | 8      | 8     |
| 2:A:1755:LEU:HD11 | 2:A:1758:CYS:N    | 0.69     | 2.03        | 4      | 8     |
| 2:A:1733:LEU:HD13 | 2:A:1733:LEU:H    | 0.65     | 1.51        | 3      | 1     |
| 1:B:131:ASN:OD1   | 1:B:134:ILE:HG13  | 0.65     | 1.91        | 15     | 1     |
| 2:A:1768:THR:HG22 | 2:A:1782:CYS:SG   | 0.64     | 2.32        | 18     | 5     |
| 2:A:1755:LEU:HD11 | 2:A:1758:CYS:CB   | 0.63     | 2.24        | 4      | 8     |
| 2:A:1755:LEU:HD12 | 2:A:1758:CYS:H    | 0.63     | 1.54        | 11     | 12    |
| 2:A:1733:LEU:O    | 2:A:1737:ARG:HG2  | 0.63     | 1.94        | 18     | 17    |
| 2:A:1755:LEU:HD12 | 2:A:1755:LEU:C    | 0.62     | 2.20        | 5      | 12    |
| 1:B:127:GLU:HA    | 2:A:1731:ARG:NH2  | 0.60     | 2.11        | 2      | 2     |
| 2:A:1765:VAL:HG13 | 2:A:1804:PRO:HG3  | 0.60     | 1.72        | 5      | 7     |
| 2:A:1732:ARG:O    | 2:A:1736:GLN:HG3  | 0.58     | 1.99        | 7      | 9     |
| 2:A:1743:VAL:O    | 2:A:1747:GLN:HG3  | 0.58     | 1.98        | 13     | 1     |
| 2:A:1739:ILE:O    | 2:A:1743:VAL:HG12 | 0.57     | 1.99        | 1      | 19    |
| 2:A:1774:LYS:HD3  | 2:A:1782:CYS:SG   | 0.56     | 2.40        | 14     | 5     |
| 1:B:131:ASN:OD1   | 2:A:1783:LYS:HE3  | 0.56     | 2.00        | 13     | 3     |
| 1:B:127:GLU:HA    | 2:A:1731:ARG:NH1  | 0.56     | 2.15        | 20     | 2     |
| 2:A:1766:GLN:HA   | 2:A:1769:LYS:CD   | 0.55     | 2.31        | 4      | 1     |
| 2:A:1767:HIS:O    | 2:A:1771:CYS:HB2  | 0.55     | 2.01        | 15     | 4     |
| 2:A:1728:GLY:O    | 2:A:1732:ARG:HB2  | 0.55     | 2.01        | 20     | 4     |
| 2:A:1782:CYS:CA   | 2:A:1785:LEU:HD12 | 0.55     | 2.31        | 13     | 10    |
| 2:A:1807:LEU:H    | 2:A:1807:LEU:HD22 | 0.55     | 1.61        | 8      | 1     |
| 2:A:1764:VAL:O    | 2:A:1768:THR:HG23 | 0.55     | 2.02        | 19     | 5     |
| 2:A:1731:ARG:NH1  | 2:A:1735:ILE:HD11 | 0.55     | 2.17        | 8      | 5     |
| 2:A:1731:ARG:HD2  | 2:A:1731:ARG:C    | 0.54     | 2.28        | 20     | 9     |
| 2:A:1768:THR:CG2  | 2:A:1785:LEU:HD13 | 0.54     | 2.32        | 14     | 11    |
| 2:A:1755:LEU:CD1  | 2:A:1755:LEU:C    | 0.53     | 2.82        | 8      | 8     |
| 2:A:1779:CYS:HB3  | 2:A:1782:CYS:HB2  | 0.53     | 1.81        | 4      | 12    |
| 2:A:1790:ALA:O    | 2:A:1794:LYS:HG2  | 0.52     | 2.04        | 17     | 10    |
| 1:B:131:ASN:HD22  | 2:A:1784:GLN:HG3  | 0.52     | 1.64        | 1      | 2     |
| 2:A:1759:GLN:NE2  | 2:A:1760:LYS:H    | 0.52     | 2.02        | 6      | 4     |
| 2:A:1733:LEU:O    | 2:A:1737:ARG:HG3  | 0.51     | 2.06        | 17     | 1     |

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| Atom-1            | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-------------------|-------------------|----------|-------------|--------|-------|
|                   |                   |          |             | Worst  | Total |
| 1:B:126:LEU:HD13  | 1:B:130:TYR:HA    | 0.51     | 1.82        | 1      | 2     |
| 2:A:1759:GLN:O    | 2:A:1763:ARG:HD3  | 0.51     | 2.06        | 5      | 5     |
| 2:A:1733:LEU:HD12 | 2:A:1734:SER:N    | 0.51     | 2.20        | 6      | 10    |
| 1:B:126:LEU:O     | 1:B:130:TYR:HB3   | 0.51     | 2.05        | 4      | 4     |
| 2:A:1773:ARG:O    | 2:A:1778:GLY:HA3  | 0.51     | 2.05        | 20     | 2     |
| 2:A:1755:LEU:CD2  | 2:A:1758:CYS:H    | 0.51     | 2.18        | 10     | 4     |
| 2:A:1755:LEU:HD11 | 2:A:1758:CYS:CA   | 0.51     | 2.35        | 4      | 5     |
| 2:A:1774:LYS:HD2  | 2:A:1782:CYS:SG   | 0.51     | 2.46        | 8      | 2     |
| 2:A:1764:VAL:O    | 2:A:1767:HIS:HB3  | 0.50     | 2.06        | 10     | 4     |
| 2:A:1768:THR:HG22 | 2:A:1785:LEU:HD13 | 0.50     | 1.83        | 7      | 6     |
| 2:A:1807:LEU:N    | 2:A:1807:LEU:HD12 | 0.50     | 2.21        | 4      | 11    |
| 2:A:1736:GLN:O    | 2:A:1740:GLN:HG3  | 0.50     | 2.07        | 14     | 5     |
| 2:A:1735:ILE:HG12 | 2:A:1788:LEU:HD12 | 0.50     | 1.84        | 13     | 2     |
| 2:A:1774:LYS:HB3  | 2:A:1779:CYS:HB3  | 0.50     | 1.84        | 18     | 1     |
| 1:B:131:ASN:ND2   | 2:A:1784:GLN:HG3  | 0.50     | 2.22        | 1      | 2     |
| 2:A:1766:GLN:O    | 2:A:1769:LYS:HB2  | 0.49     | 2.07        | 5      | 1     |
| 1:B:130:TYR:CE2   | 2:A:1784:GLN:HG2  | 0.49     | 2.42        | 14     | 1     |
| 2:A:1759:GLN:HE22 | 2:A:1760:LYS:HG2  | 0.49     | 1.66        | 12     | 5     |
| 2:A:1803:VAL:HG22 | 2:A:1806:CYS:HB2  | 0.49     | 1.83        | 13     | 2     |
| 2:A:1730:SER:O    | 2:A:1733:LEU:HD22 | 0.49     | 2.07        | 3      | 1     |
| 2:A:1755:LEU:CD1  | 2:A:1758:CYS:H    | 0.48     | 2.21        | 18     | 9     |
| 2:A:1766:GLN:HA   | 2:A:1769:LYS:HD3  | 0.48     | 1.84        | 6      | 8     |
| 2:A:1781:ILE:HG22 | 2:A:1785:LEU:HD11 | 0.48     | 1.84        | 7      | 4     |
| 2:A:1739:ILE:HD13 | 2:A:1792:HIS:HB2  | 0.48     | 1.85        | 12     | 11    |
| 2:A:1773:ARG:O    | 2:A:1773:ARG:HD3  | 0.48     | 2.08        | 19     | 1     |
| 2:A:1743:VAL:HG23 | 2:A:1802:PRO:CB   | 0.47     | 2.40        | 8      | 6     |
| 2:A:1745:ALA:CB   | 2:A:1761:MET:HB3  | 0.47     | 2.38        | 2      | 2     |
| 2:A:1765:VAL:O    | 2:A:1769:LYS:HD3  | 0.47     | 2.10        | 5      | 5     |
| 2:A:1755:LEU:HD21 | 2:A:1758:CYS:N    | 0.47     | 2.19        | 8      | 3     |
| 2:A:1759:GLN:NE2  | 2:A:1760:LYS:HG2  | 0.46     | 2.24        | 12     | 6     |
| 2:A:1755:LEU:HB2  | 2:A:1756:PRO:HD2  | 0.46     | 1.86        | 1      | 17    |
| 2:A:1755:LEU:HB2  | 2:A:1756:PRO:CD   | 0.46     | 2.41        | 11     | 4     |
| 2:A:1755:LEU:CG   | 2:A:1758:CYS:HB3  | 0.46     | 2.40        | 10     | 7     |
| 2:A:1767:HIS:NE2  | 2:A:1781:ILE:HB   | 0.46     | 2.25        | 9      | 2     |
| 2:A:1796:CYS:SG   | 2:A:1797:GLN:N    | 0.46     | 2.88        | 13     | 1     |
| 2:A:1755:LEU:C    | 2:A:1755:LEU:CD1  | 0.46     | 2.89        | 18     | 12    |
| 2:A:1745:ALA:O    | 2:A:1762:LYS:HE2  | 0.45     | 2.11        | 4      | 4     |
| 2:A:1785:LEU:HD23 | 2:A:1804:PRO:HG2  | 0.45     | 1.87        | 16     | 1     |
| 2:A:1755:LEU:HG   | 2:A:1758:CYS:CB   | 0.45     | 2.42        | 13     | 10    |
| 2:A:1782:CYS:HA   | 2:A:1785:LEU:CD1  | 0.45     | 2.36        | 19     | 1     |
| 2:A:1730:SER:HA   | 2:A:1733:LEU:HD11 | 0.45     | 1.89        | 3      | 1     |

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| Atom-1            | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-------------------|-------------------|----------|-------------|--------|-------|
|                   |                   |          |             | Worst  | Total |
| 2:A:1768:THR:HG21 | 2:A:1785:LEU:CD2  | 0.45     | 2.41        | 5      | 1     |
| 2:A:1772:LYS:O    | 2:A:1775:THR:HG22 | 0.45     | 2.12        | 1      | 2     |
| 2:A:1755:LEU:HG   | 2:A:1758:CYS:HB3  | 0.45     | 1.89        | 13     | 6     |
| 2:A:1766:GLN:HA   | 2:A:1769:LYS:HD2  | 0.44     | 1.89        | 4      | 1     |
| 2:A:1749:ARG:NE   | 2:A:1749:ARG:HA   | 0.44     | 2.26        | 19     | 1     |
| 1:B:131:ASN:OD1   | 1:B:134:ILE:HG23  | 0.44     | 2.12        | 7      | 1     |
| 1:B:129:SER:O     | 1:B:131:ASN:N     | 0.44     | 2.50        | 18     | 1     |
| 2:A:1755:LEU:O    | 2:A:1759:GLN:HG2  | 0.44     | 2.13        | 2      | 1     |
| 2:A:1766:GLN:HA   | 2:A:1769:LYS:HG2  | 0.43     | 1.88        | 17     | 1     |
| 2:A:1772:LYS:HD2  | 2:A:1772:LYS:O    | 0.43     | 2.13        | 8      | 1     |
| 2:A:1769:LYS:N    | 2:A:1769:LYS:HD2  | 0.43     | 2.28        | 13     | 1     |
| 1:B:131:ASN:O     | 1:B:134:ILE:HG12  | 0.43     | 2.13        | 5      | 1     |
| 2:A:1774:LYS:HB3  | 2:A:1779:CYS:HB2  | 0.43     | 1.90        | 4      | 2     |
| 1:B:131:ASN:HB3   | 2:A:1784:GLN:HG3  | 0.42     | 1.90        | 14     | 1     |
| 1:B:127:GLU:O     | 2:A:1731:ARG:HD3  | 0.42     | 2.14        | 18     | 1     |
| 2:A:1763:ARG:N    | 2:A:1763:ARG:HD2  | 0.42     | 2.29        | 18     | 1     |
| 1:B:130:TYR:O     | 1:B:131:ASN:HB2   | 0.42     | 2.14        | 3      | 1     |
| 2:A:1750:ASN:ND2  | 2:A:1753:CYS:HB2  | 0.42     | 2.29        | 3      | 2     |
| 1:B:131:ASN:HB3   | 1:B:134:ILE:HD11  | 0.42     | 1.92        | 15     | 1     |
| 2:A:1731:ARG:CZ   | 2:A:1735:ILE:HD11 | 0.42     | 2.45        | 17     | 1     |
| 2:A:1757:SER:O    | 2:A:1761:MET:HB2  | 0.42     | 2.15        | 2      | 1     |
| 1:B:131:ASN:O     | 1:B:134:ILE:HG13  | 0.42     | 2.15        | 3      | 1     |
| 2:A:1774:LYS:HD3  | 2:A:1782:CYS:HB2  | 0.42     | 1.91        | 5      | 1     |
| 2:A:1735:ILE:HG23 | 2:A:1788:LEU:HG   | 0.42     | 1.92        | 19     | 1     |
| 2:A:1742:LEU:HG   | 2:A:1803:VAL:HB   | 0.42     | 1.90        | 20     | 3     |
| 2:A:1759:GLN:HE21 | 2:A:1760:LYS:HG2  | 0.42     | 1.74        | 19     | 2     |
| 2:A:1731:ARG:O    | 2:A:1735:ILE:HG13 | 0.42     | 2.14        | 17     | 1     |
| 2:A:1755:LEU:HD22 | 2:A:1756:PRO:CD   | 0.41     | 2.45        | 10     | 1     |
| 2:A:1772:LYS:C    | 2:A:1774:LYS:H    | 0.41     | 2.22        | 13     | 1     |
| 2:A:1807:LEU:HD22 | 2:A:1807:LEU:N    | 0.41     | 2.30        | 8      | 1     |
| 2:A:1731:ARG:HD2  | 2:A:1732:ARG:N    | 0.41     | 2.31        | 18     | 1     |
| 1:B:134:ILE:HD13  | 2:A:1784:GLN:CD   | 0.41     | 2.39        | 1      | 1     |
| 2:A:1728:GLY:O    | 2:A:1731:ARG:HG3  | 0.41     | 2.16        | 12     | 1     |
| 2:A:1774:LYS:HD2  | 2:A:1782:CYS:CB   | 0.41     | 2.46        | 12     | 2     |
| 2:A:1731:ARG:HD3  | 2:A:1731:ARG:C    | 0.41     | 2.41        | 19     | 1     |
| 2:A:1799:ASN:HB2  | 2:A:1801:CYS:SG   | 0.41     | 2.56        | 19     | 1     |
| 2:A:1774:LYS:HD3  | 2:A:1782:CYS:CB   | 0.41     | 2.45        | 17     | 1     |
| 2:A:1727:PRO:HB2  | 2:A:1730:SER:OG   | 0.41     | 2.16        | 5      | 1     |
| 2:A:1781:ILE:HG22 | 2:A:1785:LEU:CD1  | 0.41     | 2.45        | 7      | 1     |
| 2:A:1738:ALA:O    | 2:A:1761:MET:HE2  | 0.41     | 2.16        | 11     | 2     |
| 2:A:1791:TYR:O    | 2:A:1794:LYS:HB2  | 0.41     | 2.16        | 16     | 1     |

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| Atom-1            | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-------------------|------------------|----------|-------------|--------|-------|
|                   |                  |          |             | Worst  | Total |
| 2:A:1807:LEU:O    | 2:A:1811:GLN:HG3 | 0.40     | 2.16        | 1      | 1     |
| 2:A:1778:GLY:O    | 2:A:1780:PRO:HD3 | 0.40     | 2.16        | 4      | 1     |
| 1:B:128:SER:HA    | 2:A:1731:ARG:CZ  | 0.40     | 2.45        | 18     | 1     |
| 1:B:127:GLU:O     | 2:A:1731:ARG:HG2 | 0.40     | 2.16        | 16     | 1     |
| 2:A:1735:ILE:HG12 | 2:A:1788:LEU:CD1 | 0.40     | 2.47        | 19     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed     | Outliers    | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|-------------|-------------|----|
| 1   | B     | 9/34 (26%)      | 7±0 (74±5%)  | 1±1 (16±8%) | 1±1 (10±7%) | 1           | 9  |
| 2   | A     | 85/92 (92%)     | 77±2 (91±2%) | 6±2 (7±2%)  | 1±1 (2±1%)  | 10          | 55 |
| All | All   | 1880/2520 (75%) | 1681 (89%)   | 154 (8%)    | 45 (2%)     | 7           | 44 |

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res  | Type | Models (Total) |
|-----|-------|------|------|----------------|
| 2   | A     | 1802 | PRO  | 18             |
| 1   | B     | 131  | ASN  | 14             |
| 2   | A     | 1756 | PRO  | 8              |
| 1   | B     | 129  | SER  | 2              |
| 1   | B     | 130  | TYR  | 2              |
| 2   | A     | 1772 | LYS  | 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   | B     | 9/30 (30%)      | 9±1 (96±6%)  | 0±1 (4±6%)   | 27 77       |
| 2   | A     | 73/78 (94%)     | 62±2 (86±2%) | 10±2 (14±2%) | 5 43        |
| All | All   | 1640/2160 (76%) | 1422 (87%)   | 218 (13%)    | 6 46        |

All 28 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   | A     | 1755 | LEU  | 20             |
| 2   | A     | 1764 | VAL  | 20             |
| 2   | A     | 1788 | LEU  | 20             |
| 2   | A     | 1803 | VAL  | 20             |
| 2   | A     | 1809 | ILE  | 19             |
| 2   | A     | 1767 | HIS  | 18             |
| 2   | A     | 1739 | ILE  | 17             |
| 2   | A     | 1731 | ARG  | 15             |
| 2   | A     | 1759 | GLN  | 14             |
| 2   | A     | 1801 | CYS  | 12             |
| 2   | A     | 1773 | ARG  | 5              |
| 1   | B     | 130  | TYR  | 5              |
| 2   | A     | 1772 | LYS  | 4              |
| 2   | A     | 1769 | LYS  | 4              |
| 2   | A     | 1763 | ARG  | 3              |
| 2   | A     | 1792 | HIS  | 3              |
| 2   | A     | 1784 | GLN  | 3              |
| 1   | B     | 134  | ILE  | 3              |
| 2   | A     | 1752 | ASN  | 2              |
| 2   | A     | 1797 | GLN  | 2              |
| 2   | A     | 1747 | GLN  | 2              |
| 2   | A     | 1761 | MET  | 1              |
| 2   | A     | 1733 | LEU  | 1              |
| 2   | A     | 1779 | CYS  | 1              |
| 2   | A     | 1783 | LYS  | 1              |
| 2   | A     | 1774 | LYS  | 1              |
| 2   | A     | 1771 | CYS  | 1              |
| 2   | A     | 1800 | LYS  | 1              |

### 6.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 86% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

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

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1435 |
| Number of shifts mapped to atoms        | 1435 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 126      | $-0.27 \pm 0.17$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 119      | $0.11 \pm 0.12$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 113      | $-0.22 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 115      | $-0.29 \pm 0.33$                | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1112 atoms were assigned a chemical shift out of a possible 1277. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 451/464 (97%) | 185/187 (99%) | 177/188 (94%)   | 89/89 (100%)    |
| Sidechain | 631/756 (83%) | 415/488 (85%) | 202/227 (89%)   | 14/41 (34%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 30/57 (53%)     | 18/29 (62%)          | 12/23 (52%)           | 0/5 (0%)              |
| Overall  | 1112/1277 (87%) | 618/704 (88%)        | 391/438 (89%)         | 103/135 (76%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1434 atoms were assigned a chemical shift out of a possible 1659. 0 out of 14 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  | 599/625 (96%)   | 245/253 (97%)        | 239/252 (95%)         | 115/120 (96%)         |
| Sidechain | 805/977 (82%)   | 528/633 (83%)        | 261/297 (88%)         | 16/47 (34%)           |
| Aromatic  | 30/57 (53%)     | 18/29 (62%)          | 12/23 (52%)           | 0/5 (0%)              |
| Overall   | 1434/1659 (86%) | 791/915 (86%)        | 512/572 (90%)         | 131/172 (76%)         |

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

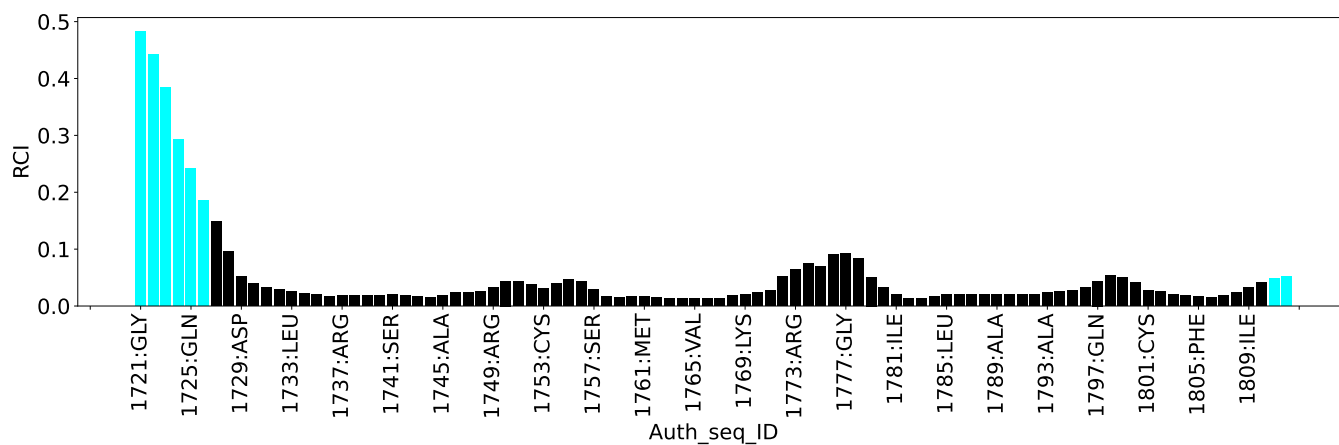
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res  | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|------|------|------|------------|---------------------|---------|
| 1       | A     | 1768 | THR  | HG1  | 5.44       | 0.08 – 2.19         | 20.4    |

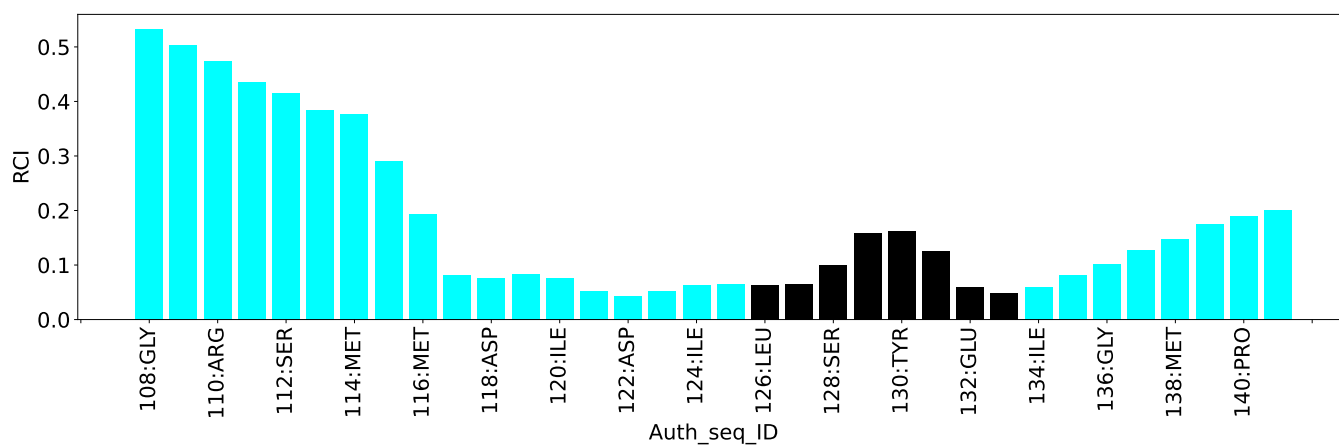
#### 7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



## 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                                | 1873  |
| Intra-residue ( $ i-j =0$ )                              | 946   |
| Sequential ( $ i-j =1$ )                                 | 410   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 257   |
| Long range ( $ i-j \geq 5$ )                             | 155   |
| Inter-chain                                              | 15    |
| Hydrogen bond restraints                                 | 90    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 190   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 16.0  |
| Number of long range restraints per residue <sup>1</sup> | 1.2   |

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 70.5                                   | 0.2     |
| 0.2-0.5 (Medium) | 116.7                                  | 0.5     |
| >0.5 (Large)     | 140.5                                  | 4.27    |

### 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)   | 4.6                                    | 5.05    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

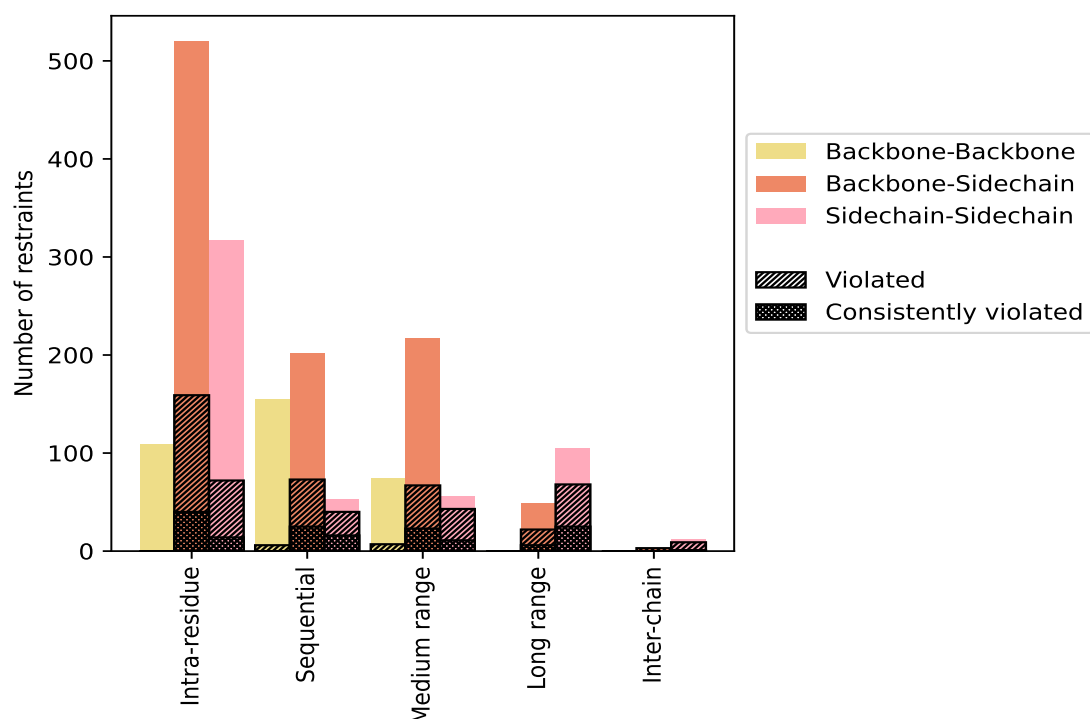
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>946</b>  | <b>50.5</b>    | <b>231</b>            | <b>24.4</b>    | <b>12.3</b>    | <b>54</b>                          | <b>5.7</b>     | <b>2.9</b>     |
| Backbone-Backbone                                                           | 109         | 5.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 520         | 27.8           | 159                   | 30.6           | 8.5            | 40                                 | 7.7            | 2.1            |
| Sidechain-Sidechain                                                         | 317         | 16.9           | 72                    | 22.7           | 3.8            | 14                                 | 4.4            | 0.7            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>410</b>  | <b>21.9</b>    | <b>119</b>            | <b>29.0</b>    | <b>6.4</b>     | <b>41</b>                          | <b>10.0</b>    | <b>2.2</b>     |
| Backbone-Backbone                                                           | 155         | 8.3            | 6                     | 3.9            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 202         | 10.8           | 73                    | 36.1           | 3.9            | 25                                 | 12.4           | 1.3            |
| Sidechain-Sidechain                                                         | 53          | 2.8            | 40                    | 75.5           | 2.1            | 16                                 | 30.2           | 0.9            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>257</b>  | <b>13.7</b>    | <b>114</b>            | <b>44.4</b>    | <b>6.1</b>     | <b>34</b>                          | <b>13.2</b>    | <b>1.8</b>     |
| Backbone-Backbone                                                           | 74          | 4.0            | 7                     | 9.5            | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 127         | 6.8            | 64                    | 50.4           | 3.4            | 23                                 | 18.1           | 1.2            |
| Sidechain-Sidechain                                                         | 56          | 3.0            | 43                    | 76.8           | 2.3            | 11                                 | 19.6           | 0.6            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>155</b>  | <b>8.3</b>     | <b>90</b>             | <b>58.1</b>    | <b>4.8</b>     | <b>31</b>                          | <b>20.0</b>    | <b>1.7</b>     |
| Backbone-Backbone                                                           | 1           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 49          | 2.6            | 22                    | 44.9           | 1.2            | 6                                  | 12.2           | 0.3            |
| Sidechain-Sidechain                                                         | 105         | 5.6            | 68                    | 64.8           | 3.6            | 25                                 | 23.8           | 1.3            |
| <b>Inter-chain</b>                                                          | <b>15</b>   | <b>0.8</b>     | <b>12</b>             | <b>80.0</b>    | <b>0.6</b>     | <b>1</b>                           | <b>6.7</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 3           | 0.2            | 3                     | 100.0          | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 12          | 0.6            | 9                     | 75.0           | 0.5            | 1                                  | 8.3            | 0.1            |
| <b>Hydrogen bond</b>                                                        | <b>90</b>   | <b>4.8</b>     | <b>3</b>              | <b>3.3</b>     | <b>0.2</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>1873</b> | <b>100.0</b>   | <b>569</b>            | <b>30.4</b>    | <b>30.4</b>    | <b>161</b>                         | <b>8.6</b>     | <b>8.6</b>     |
| Backbone-Backbone                                                           | 339         | 18.1           | 13                    | 3.8            | 0.7            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 991         | 52.9           | 324                   | 32.7           | 17.3           | 94                                 | 9.5            | 5.0            |
| Sidechain-Sidechain                                                         | 543         | 29.0           | 232                   | 42.7           | 12.4           | 67                                 | 12.3           | 3.6            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 130                  | 72              | 67              | 55              | 3               | 327   | 0.55     | 2.58    | 0.45                | 0.43       |
| 2        | 132                  | 74              | 61              | 59              | 4               | 330   | 0.59     | 3.51    | 0.51                | 0.46       |
| 3        | 127                  | 73              | 75              | 57              | 6               | 338   | 0.57     | 2.77    | 0.48                | 0.45       |
| 4        | 128                  | 76              | 69              | 55              | 4               | 332   | 0.6      | 3.59    | 0.52                | 0.46       |
| 5        | 126                  | 76              | 62              | 64              | 3               | 331   | 0.59     | 4.27    | 0.55                | 0.44       |
| 6        | 126                  | 70              | 70              | 54              | 4               | 324   | 0.56     | 3.52    | 0.49                | 0.42       |
| 7        | 130                  | 73              | 66              | 59              | 6               | 334   | 0.58     | 2.44    | 0.47                | 0.44       |
| 8        | 134                  | 82              | 63              | 53              | 5               | 337   | 0.57     | 2.75    | 0.47                | 0.43       |
| 9        | 133                  | 77              | 71              | 53              | 4               | 338   | 0.6      | 3.33    | 0.51                | 0.46       |
| 10       | 134                  | 73              | 56              | 60              | 4               | 327   | 0.6      | 3.41    | 0.52                | 0.45       |

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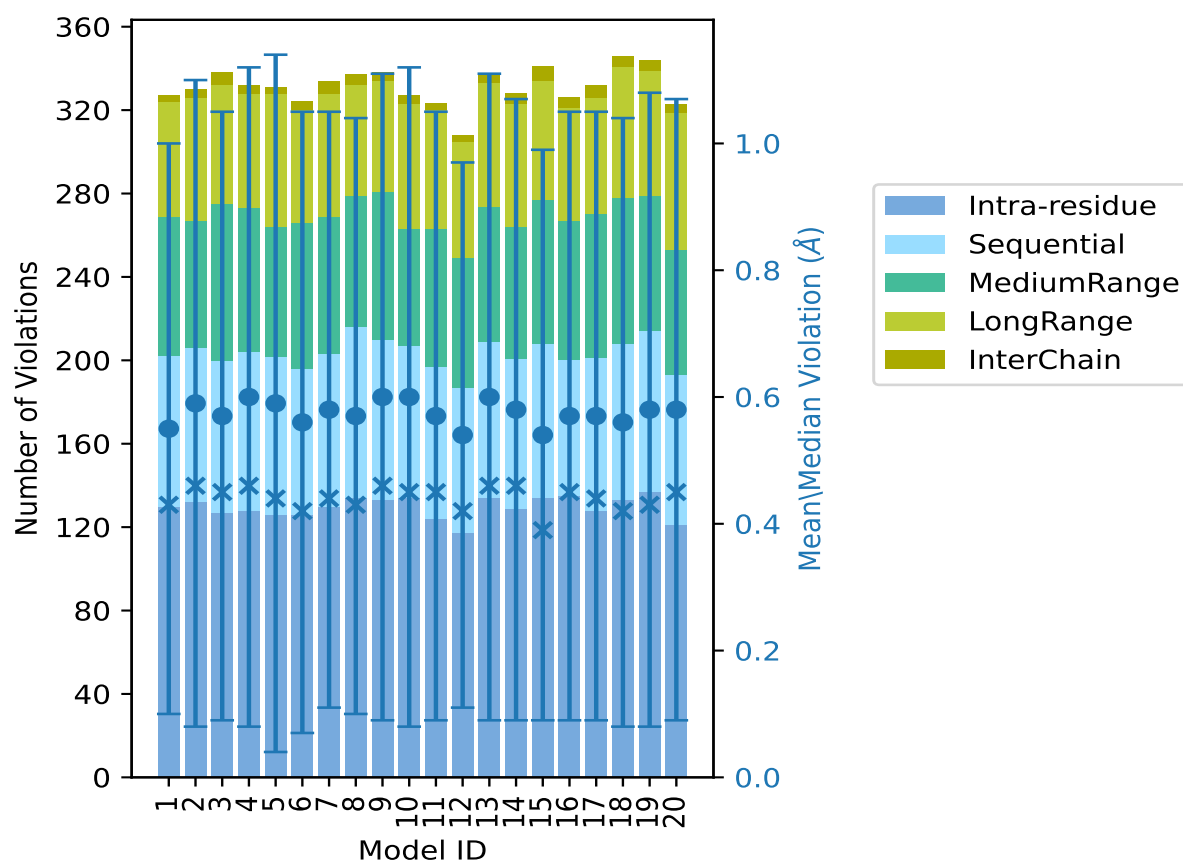
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 124                  | 73              | 66              | 57              | 3               | 323   | 0.57     | 3.62    | 0.48                | 0.45       |
| 12       | 117                  | 70              | 62              | 56              | 3               | 308   | 0.54     | 2.39    | 0.43                | 0.42       |
| 13       | 134                  | 75              | 65              | 59              | 4               | 337   | 0.6      | 3.42    | 0.51                | 0.46       |
| 14       | 129                  | 72              | 63              | 59              | 5               | 328   | 0.58     | 3.38    | 0.49                | 0.46       |
| 15       | 134                  | 74              | 69              | 57              | 7               | 341   | 0.54     | 2.52    | 0.45                | 0.39       |
| 16       | 135                  | 65              | 67              | 54              | 5               | 326   | 0.57     | 3.41    | 0.48                | 0.45       |
| 17       | 128                  | 73              | 69              | 56              | 6               | 332   | 0.57     | 3.44    | 0.48                | 0.44       |
| 18       | 133                  | 75              | 70              | 63              | 5               | 346   | 0.56     | 3.67    | 0.48                | 0.42       |
| 19       | 137                  | 77              | 65              | 60              | 5               | 344   | 0.58     | 3.61    | 0.5                 | 0.43       |
| 20       | 121                  | 72              | 60              | 66              | 4               | 323   | 0.58     | 3.39    | 0.49                | 0.45       |

<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

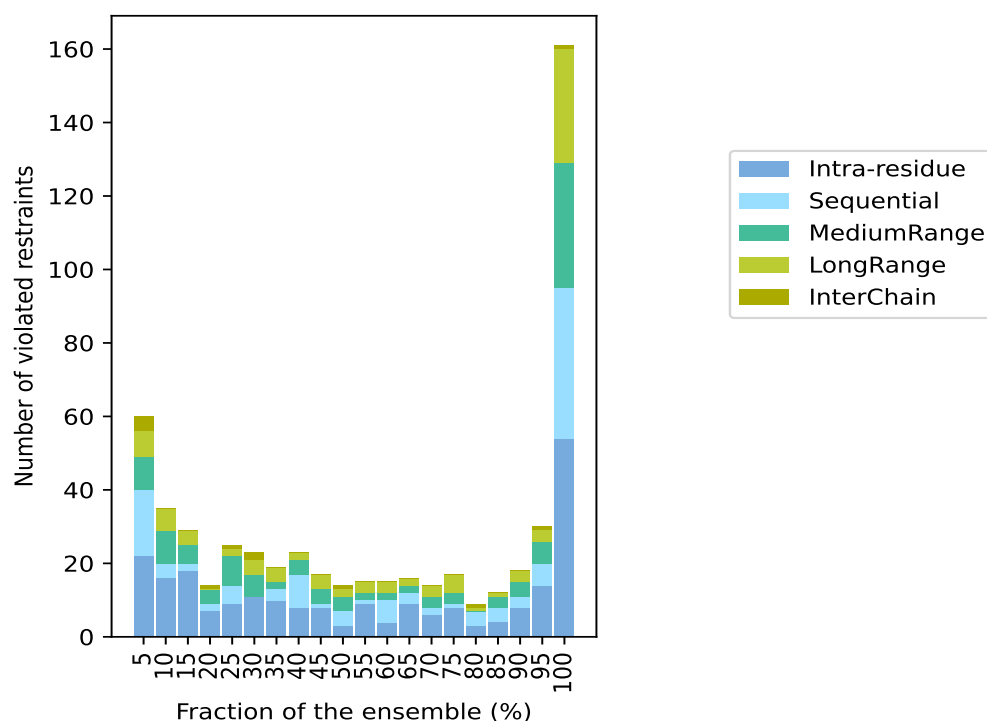
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1217(IR:715, SQ:291, MR:143, LR:65, IC:3) restraints are 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>       | %     |
| 22                            | 18              | 9               | 7               | 4               | 60    | 1                        | 5.0   |
| 16                            | 4               | 9               | 6               | 0               | 35    | 2                        | 10.0  |
| 18                            | 2               | 5               | 4               | 0               | 29    | 3                        | 15.0  |
| 7                             | 2               | 4               | 0               | 1               | 14    | 4                        | 20.0  |
| 9                             | 5               | 8               | 2               | 1               | 25    | 5                        | 25.0  |
| 11                            | 0               | 6               | 4               | 2               | 23    | 6                        | 30.0  |
| 10                            | 3               | 2               | 4               | 0               | 19    | 7                        | 35.0  |
| 8                             | 9               | 4               | 2               | 0               | 23    | 8                        | 40.0  |
| 8                             | 1               | 4               | 4               | 0               | 17    | 9                        | 45.0  |
| 3                             | 4               | 4               | 2               | 1               | 14    | 10                       | 50.0  |
| 9                             | 1               | 2               | 3               | 0               | 15    | 11                       | 55.0  |
| 4                             | 6               | 2               | 3               | 0               | 15    | 12                       | 60.0  |
| 9                             | 3               | 2               | 2               | 0               | 16    | 13                       | 65.0  |
| 6                             | 2               | 3               | 3               | 0               | 14    | 14                       | 70.0  |
| 8                             | 1               | 3               | 5               | 0               | 17    | 15                       | 75.0  |
| 3                             | 4               | 0               | 1               | 1               | 9     | 16                       | 80.0  |
| 4                             | 4               | 3               | 1               | 0               | 12    | 17                       | 85.0  |
| 8                             | 3               | 4               | 3               | 0               | 18    | 18                       | 90.0  |
| 14                            | 6               | 6               | 3               | 1               | 30    | 19                       | 95.0  |
| 54                            | 41              | 34              | 31              | 1               | 161   | 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

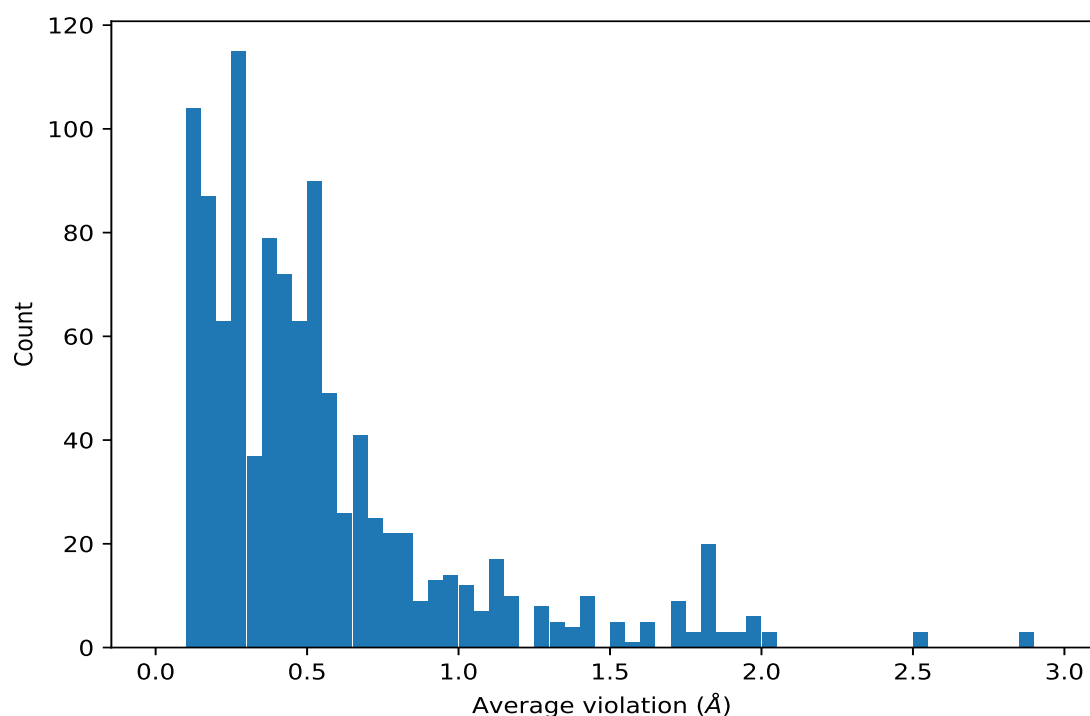
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,665)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:HG13  | 20                  | 2.9      | 0.85                | 3.41       |
| (2,665)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:HG13  | 20                  | 2.9      | 0.85                | 3.41       |
| (2,665)  | 1:119:B:VAL:HG11  | 1:120:B:ILE:HG13  | 20                  | 2.9      | 0.85                | 3.41       |
| (2,1015) | 2:1735:A:ILE:HB   | 2:1788:A:LEU:HD23 | 20                  | 2.53     | 0.13                | 2.52       |
| (2,1015) | 2:1735:A:ILE:HB   | 2:1788:A:LEU:HD21 | 20                  | 2.53     | 0.13                | 2.52       |
| (2,1015) | 2:1735:A:ILE:HB   | 2:1788:A:LEU:HD22 | 20                  | 2.53     | 0.13                | 2.52       |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 20                  | 1.96     | 0.06                | 1.97       |
| (2,1634) | 2:1788:A:LEU:HD22 | 2:1791:A:TYR:HD1  | 20                  | 1.96     | 0.06                | 1.97       |
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD2  | 20                  | 1.96     | 0.06                | 1.97       |
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD1  | 20                  | 1.96     | 0.06                | 1.97       |
| (2,1634) | 2:1788:A:LEU:HD22 | 2:1791:A:TYR:HD2  | 20                  | 1.96     | 0.06                | 1.97       |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD1  | 20                  | 1.96     | 0.06                | 1.97       |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 20                  | 1.95     | 0.41                | 2.1        |
| (2,561)  | 1:119:B:VAL:HG23  | 1:118:B:ASP:HB3   | 20                  | 1.95     | 0.41                | 2.1        |
| (2,561)  | 1:119:B:VAL:HG22  | 1:118:B:ASP:HB3   | 20                  | 1.95     | 0.41                | 2.1        |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 20                  | 1.84     | 0.01                | 1.84       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD21 | 20                  | 1.84     | 0.01                | 1.84       |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 20                  | 1.84     | 0.01                | 1.84       |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD11 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD13 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD12 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD13 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD11 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD11 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD12 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD12 | 20                  | 1.82     | 0.25                | 1.85       |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 20                  | 1.82     | 0.19                | 1.81       |
| (2,1404) | 2:1788:A:LEU:HD12 | 2:1739:A:ILE:H    | 20                  | 1.82     | 0.19                | 1.81       |
| (2,1404) | 2:1788:A:LEU:HD13 | 2:1739:A:ILE:H    | 20                  | 1.82     | 0.19                | 1.81       |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 20                  | 1.81     | 0.04                | 1.82       |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD23 | 20                  | 1.81     | 0.04                | 1.82       |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD21 | 20                  | 1.81     | 0.04                | 1.82       |
| (2,1500) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HD3  | 20                  | 1.81     | 0.15                | 1.81       |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 20                  | 1.81     | 0.15                | 1.81       |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 20                  | 1.81     | 0.15                | 1.81       |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD11 | 20                  | 1.75     | 0.04                | 1.75       |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 20                  | 1.75     | 0.04                | 1.75       |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD13 | 20                  | 1.75     | 0.04                | 1.75       |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 20                  | 1.74     | 0.03                | 1.74       |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 20                  | 1.74     | 0.03                | 1.74       |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 20                  | 1.72     | 0.11                | 1.71       |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD21 | 20                  | 1.72     | 0.11                | 1.71       |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 20                  | 1.72     | 0.11                | 1.71       |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 20                  | 1.71     | 0.23                | 1.67       |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 20                  | 1.71     | 0.23                | 1.67       |
| (2,1402) | 2:1788:A:LEU:HD13 | 2:1785:A:LEU:HA   | 20                  | 1.71     | 0.23                | 1.67       |
| (2,1359) | 2:1742:A:LEU:HD13 | 2:1739:A:ILE:HA   | 20                  | 1.62     | 0.12                | 1.64       |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 20                  | 1.62     | 0.12                | 1.64       |
| (2,1359) | 2:1742:A:LEU:HD11 | 2:1739:A:ILE:HA   | 20                  | 1.62     | 0.12                | 1.64       |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 20                  | 1.53     | 0.07                | 1.52       |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 20                  | 1.38     | 0.56                | 1.62       |
| (2,1304) | 2:1751:A:ALA:HB1  | 2:1752:A:ASN:HB2  | 20                  | 1.38     | 0.56                | 1.62       |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 20                  | 1.38     | 0.56                | 1.62       |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 20                  | 1.37     | 0.09                | 1.39       |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 20                  | 1.34     | 0.16                | 1.43       |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 20                  | 1.3      | 0.02                | 1.31       |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 20                  | 1.3      | 0.02                | 1.31       |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 20                  | 1.26     | 0.07                | 1.26       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 20                  | 1.2      | 0.09                | 1.19       |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 20                  | 1.18     | 0.04                | 1.18       |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG13 | 20                  | 1.18     | 0.04                | 1.18       |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG12 | 20                  | 1.18     | 0.04                | 1.18       |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 20                  | 1.15     | 0.18                | 1.14       |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 20                  | 1.13     | 0.11                | 1.12       |
| (2,1693) | 2:1755:A:LEU:HD12 | 2:1754:A:SER:HB2  | 20                  | 1.1      | 0.46                | 0.85       |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 20                  | 1.1      | 0.46                | 0.85       |
| (2,1693) | 2:1755:A:LEU:HD11 | 2:1754:A:SER:HB2  | 20                  | 1.1      | 0.46                | 0.85       |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 20                  | 1.1      | 0.45                | 1.43       |
| (2,752)  | 2:1785:A:LEU:HD22 | 2:1786:A:ILE:H    | 20                  | 1.1      | 0.45                | 1.43       |
| (2,752)  | 2:1785:A:LEU:HD21 | 2:1786:A:ILE:H    | 20                  | 1.1      | 0.45                | 1.43       |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 20                  | 1.07     | 0.65                | 1.42       |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD22 | 20                  | 1.07     | 0.65                | 1.42       |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD21 | 20                  | 1.07     | 0.65                | 1.42       |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 20                  | 1.06     | 0.06                | 1.07       |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 20                  | 1.06     | 0.13                | 1.04       |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 20                  | 1.03     | 0.04                | 1.02       |
| (2,1687) | 2:1745:A:ALA:HB2  | 2:1762:A:LYS:HB3  | 20                  | 1.0      | 0.03                | 1.0        |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3  | 20                  | 1.0      | 0.03                | 1.0        |
| (2,1687) | 2:1745:A:ALA:HB1  | 2:1762:A:LYS:HB3  | 20                  | 1.0      | 0.03                | 1.0        |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 20                  | 0.98     | 0.23                | 0.96       |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 20                  | 0.98     | 0.69                | 1.5        |
| (2,922)  | 2:1765:A:VAL:HG22 | 2:1804:A:PRO:HG2  | 20                  | 0.98     | 0.69                | 1.5        |
| (2,922)  | 2:1765:A:VAL:HG23 | 2:1804:A:PRO:HG2  | 20                  | 0.98     | 0.69                | 1.5        |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA   | 20                  | 0.97     | 0.02                | 0.98       |
| (2,1027) | 2:1742:A:LEU:HD22 | 2:1803:A:VAL:HA   | 20                  | 0.97     | 0.02                | 0.98       |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA   | 20                  | 0.97     | 0.02                | 0.98       |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 20                  | 0.97     | 0.44                | 1.15       |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 20                  | 0.97     | 0.44                | 1.15       |
| (2,1133) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:HG2  | 20                  | 0.97     | 0.44                | 1.15       |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB1  | 20                  | 0.91     | 0.2                 | 0.95       |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2  | 20                  | 0.91     | 0.2                 | 0.95       |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB3  | 20                  | 0.91     | 0.2                 | 0.95       |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 20                  | 0.88     | 0.09                | 0.9        |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 20                  | 0.86     | 0.01                | 0.86       |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 20                  | 0.86     | 0.01                | 0.86       |
| (2,1361) | 2:1742:A:LEU:HD12 | 2:1742:A:LEU:HB3  | 20                  | 0.86     | 0.01                | 0.86       |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 20                  | 0.86     | 0.02                | 0.86       |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 20                  | 0.83     | 0.02                | 0.84       |
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3  | 20                  | 0.83     | 0.14                | 0.86       |
| (2,1396) | 2:1793:A:ALA:HB3  | 2:1796:A:CYS:HB3  | 20                  | 0.83     | 0.14                | 0.86       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 20                  | 0.83     | 0.14                | 0.86       |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB2  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB1  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB2  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB2  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB3  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB3  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB1  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB1  | 20                  | 0.83     | 0.06                | 0.82       |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 20                  | 0.81     | 0.03                | 0.81       |
| (2,1554) | 2:1735:A:ILE:HD11 | 2:1791:A:TYR:HE2  | 20                  | 0.8      | 0.05                | 0.8        |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE2  | 20                  | 0.8      | 0.05                | 0.8        |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE1  | 20                  | 0.8      | 0.05                | 0.8        |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE1  | 20                  | 0.8      | 0.05                | 0.8        |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE2  | 20                  | 0.8      | 0.05                | 0.8        |
| (2,1554) | 2:1735:A:ILE:HD11 | 2:1791:A:TYR:HE1  | 20                  | 0.8      | 0.05                | 0.8        |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 20                  | 0.79     | 0.19                | 0.76       |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 20                  | 0.79     | 0.19                | 0.76       |
| (2,1120) | 2:1739:A:ILE:HG22 | 2:1792:A:HIS:HB3  | 20                  | 0.79     | 0.19                | 0.76       |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD1   | 20                  | 0.78     | 0.35                | 0.85       |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD2   | 20                  | 0.78     | 0.35                | 0.85       |
| (2,1148) | 2:1788:A:LEU:HD21 | 1:130:B:TYR:HD1   | 20                  | 0.78     | 0.35                | 0.85       |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD1   | 20                  | 0.78     | 0.35                | 0.85       |
| (2,1148) | 2:1788:A:LEU:HD21 | 1:130:B:TYR:HD2   | 20                  | 0.78     | 0.35                | 0.85       |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD2   | 20                  | 0.78     | 0.35                | 0.85       |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 20                  | 0.78     | 0.17                | 0.77       |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 20                  | 0.77     | 0.12                | 0.7        |
| (2,1186) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD2  | 20                  | 0.77     | 0.12                | 0.7        |
| (2,1186) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD2  | 20                  | 0.77     | 0.12                | 0.7        |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB2  | 20                  | 0.76     | 0.04                | 0.76       |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 20                  | 0.76     | 0.04                | 0.76       |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB1  | 20                  | 0.76     | 0.04                | 0.76       |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 20                  | 0.76     | 0.01                | 0.76       |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 20                  | 0.74     | 0.03                | 0.74       |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE2  | 20                  | 0.74     | 0.03                | 0.74       |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE3  | 20                  | 0.74     | 0.03                | 0.74       |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 20                  | 0.74     | 0.12                | 0.77       |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 20                  | 0.73     | 0.09                | 0.77       |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG13 | 20                  | 0.73     | 0.09                | 0.77       |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG12 | 20                  | 0.73     | 0.09                | 0.77       |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 20                  | 0.72     | 0.03                | 0.72       |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 20                  | 0.7      | 0.12                | 0.64       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 20                  | 0.68     | 0.03                | 0.68       |
| (2,632)  | 1:119:B:VAL:HG22  | 1:119:B:VAL:HA    | 20                  | 0.68     | 0.03                | 0.68       |
| (2,632)  | 1:119:B:VAL:HG21  | 1:119:B:VAL:HA    | 20                  | 0.68     | 0.03                | 0.68       |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG21 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG23 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG21 | 2:1781:A:ILE:HG21 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG23 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG22 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG21 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG22 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG21 | 2:1781:A:ILE:HG23 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1084) | 2:1768:A:THR:HG21 | 2:1781:A:ILE:HG22 | 20                  | 0.67     | 0.09                | 0.71       |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 20                  | 0.66     | 0.28                | 0.82       |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 20                  | 0.66     | 0.12                | 0.67       |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 20                  | 0.65     | 0.07                | 0.65       |
| (2,1442) | 2:1790:A:ALA:HB2  | 2:1791:A:TYR:HB2  | 20                  | 0.65     | 0.07                | 0.65       |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 20                  | 0.65     | 0.07                | 0.65       |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 20                  | 0.65     | 0.04                | 0.64       |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB2  | 20                  | 0.65     | 0.04                | 0.64       |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB1  | 20                  | 0.65     | 0.04                | 0.64       |
| (2,1364) | 2:1742:A:LEU:HD11 | 2:1743:A:VAL:H    | 20                  | 0.64     | 0.03                | 0.64       |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 20                  | 0.64     | 0.03                | 0.64       |
| (2,1364) | 2:1742:A:LEU:HD12 | 2:1743:A:VAL:H    | 20                  | 0.64     | 0.03                | 0.64       |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 20                  | 0.64     | 0.11                | 0.66       |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 20                  | 0.63     | 0.03                | 0.63       |
| (3,12)   | 1:123:B:ILE:HA    | 1:126:B:LEU:HD22  | 20                  | 0.63     | 0.22                | 0.71       |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD11  | 20                  | 0.63     | 0.22                | 0.71       |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD13  | 20                  | 0.63     | 0.22                | 0.71       |
| (3,12)   | 1:123:B:ILE:HA    | 1:126:B:LEU:HD21  | 20                  | 0.63     | 0.22                | 0.71       |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD12  | 20                  | 0.63     | 0.22                | 0.71       |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG12 | 20                  | 0.62     | 0.08                | 0.62       |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG12 | 20                  | 0.62     | 0.08                | 0.62       |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG11 | 20                  | 0.62     | 0.08                | 0.62       |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG13 | 20                  | 0.62     | 0.08                | 0.62       |
| (2,725)  | 2:1746:A:ALA:HB3  | 2:1803:A:VAL:HG11 | 20                  | 0.62     | 0.08                | 0.62       |
| (2,725)  | 2:1746:A:ALA:HB3  | 2:1803:A:VAL:HG13 | 20                  | 0.62     | 0.08                | 0.62       |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG13 | 20                  | 0.62     | 0.08                | 0.62       |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 20                  | 0.59     | 0.03                | 0.6        |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 20                  | 0.59     | 0.03                | 0.6        |
| (2,1284) | 2:1786:A:ILE:HD12 | 2:1786:A:ILE:HA   | 20                  | 0.59     | 0.03                | 0.6        |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 20                  | 0.58     | 0.02                | 0.58       |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 20                  | 0.58     | 0.03                | 0.58       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 20                  | 0.58     | 0.03                | 0.58       |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG21 | 20                  | 0.58     | 0.03                | 0.58       |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 20                  | 0.57     | 0.03                | 0.57       |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD11 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD13 | 20                  | 0.56     | 0.06                | 0.56       |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 20                  | 0.55     | 0.52                | 0.46       |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD13 | 20                  | 0.55     | 0.52                | 0.46       |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 20                  | 0.55     | 0.52                | 0.46       |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 20                  | 0.55     | 0.21                | 0.68       |
| (2,1184) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD3  | 20                  | 0.55     | 0.21                | 0.68       |
| (2,1184) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD3  | 20                  | 0.55     | 0.21                | 0.68       |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG22 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG23 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG22 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG22 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG21 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG21 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG23 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG21 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG23 | 20                  | 0.54     | 0.07                | 0.55       |
| (2,1501) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 20                  | 0.54     | 0.04                | 0.54       |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB3  | 20                  | 0.54     | 0.02                | 0.54       |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 20                  | 0.54     | 0.02                | 0.54       |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB2  | 20                  | 0.54     | 0.02                | 0.54       |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 20                  | 0.54     | 0.01                | 0.54       |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 20                  | 0.54     | 0.01                | 0.54       |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG12 | 20                  | 0.53     | 0.06                | 0.53       |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG12 | 20                  | 0.53     | 0.06                | 0.53       |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG13 | 20                  | 0.53     | 0.06                | 0.53       |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG11 | 20                  | 0.53     | 0.06                | 0.53       |
| (2,726)  | 2:1746:A:ALA:HB1  | 2:1765:A:VAL:HG13 | 20                  | 0.53     | 0.06                | 0.53       |
| (2,726)  | 2:1746:A:ALA:HB1  | 2:1765:A:VAL:HG11 | 20                  | 0.53     | 0.06                | 0.53       |
| (2,726)  | 2:1746:A:ALA:HB1  | 2:1765:A:VAL:HG12 | 20                  | 0.53     | 0.06                | 0.53       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG13 | 20                  | 0.53     | 0.06                | 0.53       |
| (2,1176) | 2:1755:A:LEU:HD11 | 2:1756:A:PRO:HD3  | 20                  | 0.53     | 0.43                | 0.2        |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 20                  | 0.53     | 0.43                | 0.2        |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 20                  | 0.53     | 0.43                | 0.2        |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 20                  | 0.53     | 0.01                | 0.53       |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 20                  | 0.52     | 0.03                | 0.52       |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 20                  | 0.51     | 0.13                | 0.45       |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 20                  | 0.51     | 0.13                | 0.45       |
| (2,1526) | 2:1746:A:ALA:HB3  | 2:1804:A:PRO:HD2  | 20                  | 0.51     | 0.13                | 0.45       |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 20                  | 0.51     | 0.14                | 0.57       |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 20                  | 0.51     | 0.01                | 0.51       |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 20                  | 0.5      | 0.29                | 0.4        |
| (2,1655) | 2:1787:A:ALA:HB2  | 2:1784:A:GLN:HB3  | 20                  | 0.5      | 0.29                | 0.4        |
| (2,1655) | 2:1787:A:ALA:HB3  | 2:1784:A:GLN:HB3  | 20                  | 0.5      | 0.29                | 0.4        |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 20                  | 0.5      | 0.12                | 0.52       |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG23 | 20                  | 0.5      | 0.12                | 0.52       |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 20                  | 0.5      | 0.12                | 0.52       |
| (2,966)  | 2:1739:A:ILE:HD11 | 2:1788:A:LEU:HB2  | 20                  | 0.5      | 0.04                | 0.49       |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 20                  | 0.5      | 0.04                | 0.49       |
| (2,966)  | 2:1739:A:ILE:HD13 | 2:1788:A:LEU:HB2  | 20                  | 0.5      | 0.04                | 0.49       |
| (2,99)   | 2:1745:A:ALA:HB3  | 2:1744:A:HIS:H    | 20                  | 0.5      | 0.04                | 0.5        |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 20                  | 0.5      | 0.04                | 0.5        |
| (2,99)   | 2:1745:A:ALA:HB2  | 2:1744:A:HIS:H    | 20                  | 0.5      | 0.04                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD11 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD13 | 20                  | 0.5      | 0.06                | 0.5        |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 20                  | 0.5      | 0.02                | 0.5        |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 20                  | 0.49     | 0.13                | 0.5        |
| (2,1002) | 2:1738:A:ALA:HB3  | 2:1739:A:ILE:HA   | 20                  | 0.49     | 0.02                | 0.49       |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 20                  | 0.49     | 0.02                | 0.49       |
| (2,1002) | 2:1738:A:ALA:HB2  | 2:1739:A:ILE:HA   | 20                  | 0.49     | 0.02                | 0.49       |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 20                  | 0.49     | 0.11                | 0.52       |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 20                  | 0.48     | 0.03                | 0.48       |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 20                  | 0.48     | 0.03                | 0.48       |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG23 | 20                  | 0.48     | 0.03                | 0.48       |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 20                  | 0.48     | 0.02                | 0.48       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 20                  | 0.48     | 0.02                | 0.48       |
| (2,1518) | 2:1764:A:VAL:HG11 | 2:1766:A:GLN:H    | 20                  | 0.48     | 0.02                | 0.48       |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 20                  | 0.48     | 0.06                | 0.46       |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 20                  | 0.48     | 0.06                | 0.46       |
| (2,1710) | 2:1789:A:ALA:HB2  | 2:1790:A:ALA:HA   | 20                  | 0.48     | 0.06                | 0.46       |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 20                  | 0.48     | 0.06                | 0.48       |
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 20                  | 0.48     | 0.06                | 0.48       |
| (2,82)   | 2:1764:A:VAL:HG11 | 2:1764:A:VAL:H    | 20                  | 0.48     | 0.06                | 0.48       |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 20                  | 0.47     | 0.03                | 0.47       |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 20                  | 0.47     | 0.05                | 0.48       |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB3  | 20                  | 0.47     | 0.05                | 0.48       |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB2  | 20                  | 0.47     | 0.05                | 0.48       |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 20                  | 0.47     | 0.02                | 0.46       |
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 20                  | 0.47     | 0.02                | 0.46       |
| (2,249)  | 2:1781:A:ILE:HG22 | 2:1781:A:ILE:H    | 20                  | 0.47     | 0.02                | 0.46       |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 20                  | 0.46     | 0.05                | 0.46       |
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 20                  | 0.44     | 0.04                | 0.45       |
| (2,812)  | 2:1786:A:ILE:HG23 | 2:1783:A:LYS:HA   | 20                  | 0.44     | 0.04                | 0.45       |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 20                  | 0.44     | 0.04                | 0.45       |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 20                  | 0.44     | 0.24                | 0.36       |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 20                  | 0.44     | 0.24                | 0.36       |
| (2,1515) | 2:1764:A:VAL:HG12 | 2:1761:A:MET:HG2  | 20                  | 0.44     | 0.24                | 0.36       |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 20                  | 0.44     | 0.06                | 0.44       |
| (2,558)  | 1:120:B:ILE:HD11  | 1:120:B:ILE:H     | 20                  | 0.43     | 0.09                | 0.47       |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 20                  | 0.43     | 0.09                | 0.47       |
| (2,558)  | 1:120:B:ILE:HD12  | 1:120:B:ILE:H     | 20                  | 0.43     | 0.09                | 0.47       |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG12 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG12 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG11 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG13 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD12 | 2:1803:A:VAL:HG11 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD12 | 2:1803:A:VAL:HG13 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG13 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG11 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1358) | 2:1742:A:LEU:HD12 | 2:1803:A:VAL:HG12 | 20                  | 0.43     | 0.11                | 0.4        |
| (2,1415) | 2:1735:A:ILE:HD12 | 2:1735:A:ILE:H    | 20                  | 0.43     | 0.06                | 0.44       |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 20                  | 0.43     | 0.06                | 0.44       |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 20                  | 0.43     | 0.06                | 0.44       |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 20                  | 0.42     | 0.01                | 0.42       |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB3  | 20                  | 0.42     | 0.01                | 0.42       |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB1  | 20                  | 0.42     | 0.01                | 0.42       |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 20                  | 0.41     | 0.06                | 0.42       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1607) | 2:1781:A:ILE:HD11 | 2:1782:A:CYS:H    | 20                  | 0.41     | 0.04                | 0.42       |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 20                  | 0.41     | 0.04                | 0.42       |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 20                  | 0.41     | 0.04                | 0.42       |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 20                  | 0.41     | 0.18                | 0.54       |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 20                  | 0.41     | 0.18                | 0.54       |
| (2,1343) | 2:1755:A:LEU:HD21 | 2:1755:A:LEU:HA   | 20                  | 0.41     | 0.18                | 0.54       |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 20                  | 0.4      | 0.04                | 0.4        |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 20                  | 0.4      | 0.04                | 0.4        |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG21 | 20                  | 0.4      | 0.04                | 0.4        |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 20                  | 0.4      | 0.01                | 0.4        |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 20                  | 0.39     | 0.05                | 0.38       |
| (2,919)  | 2:1765:A:VAL:HG21 | 2:1762:A:LYS:HA   | 20                  | 0.39     | 0.05                | 0.38       |
| (2,919)  | 2:1765:A:VAL:HG22 | 2:1762:A:LYS:HA   | 20                  | 0.39     | 0.05                | 0.38       |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 20                  | 0.39     | 0.13                | 0.36       |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD22 | 20                  | 0.39     | 0.13                | 0.36       |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 20                  | 0.39     | 0.13                | 0.36       |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 20                  | 0.39     | 0.03                | 0.4        |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 20                  | 0.39     | 0.06                | 0.36       |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 20                  | 0.39     | 0.06                | 0.36       |
| (2,1085) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:H    | 20                  | 0.39     | 0.06                | 0.36       |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 20                  | 0.39     | 0.04                | 0.39       |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 20                  | 0.39     | 0.04                | 0.39       |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD11 | 20                  | 0.39     | 0.04                | 0.39       |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 20                  | 0.37     | 0.11                | 0.43       |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 20                  | 0.37     | 0.06                | 0.36       |
| (2,1130) | 2:1761:A:MET:HE2  | 2:1739:A:ILE:HA   | 20                  | 0.37     | 0.06                | 0.36       |
| (2,1130) | 2:1761:A:MET:HE3  | 2:1739:A:ILE:HA   | 20                  | 0.37     | 0.06                | 0.36       |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB3  | 20                  | 0.37     | 0.07                | 0.37       |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 20                  | 0.37     | 0.07                | 0.37       |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB2  | 20                  | 0.37     | 0.07                | 0.37       |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 20                  | 0.37     | 0.13                | 0.3        |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 20                  | 0.37     | 0.13                | 0.3        |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD21 | 20                  | 0.37     | 0.13                | 0.3        |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 20                  | 0.36     | 0.0                 | 0.36       |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 20                  | 0.32     | 0.13                | 0.33       |
| (2,1698) | 2:1788:A:LEU:HD23 | 2:1787:A:ALA:H    | 20                  | 0.32     | 0.13                | 0.33       |
| (2,1698) | 2:1788:A:LEU:HD21 | 2:1787:A:ALA:H    | 20                  | 0.32     | 0.13                | 0.33       |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG21 | 20                  | 0.32     | 0.04                | 0.32       |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 20                  | 0.32     | 0.04                | 0.32       |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 20                  | 0.32     | 0.04                | 0.32       |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 20                  | 0.32     | 0.09                | 0.32       |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 20                  | 0.32     | 0.09                | 0.32       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD13 | 20                  | 0.3      | 0.03                | 0.3        |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 20                  | 0.3      | 0.03                | 0.3        |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD12 | 20                  | 0.3      | 0.03                | 0.3        |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 20                  | 0.29     | 0.05                | 0.3        |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 20                  | 0.29     | 0.05                | 0.3        |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG13 | 20                  | 0.29     | 0.05                | 0.3        |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 20                  | 0.29     | 0.04                | 0.29       |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 20                  | 0.29     | 0.04                | 0.29       |
| (2,210)  | 2:1739:A:ILE:HG23 | 2:1739:A:ILE:H    | 20                  | 0.28     | 0.02                | 0.28       |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 20                  | 0.28     | 0.02                | 0.28       |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 20                  | 0.28     | 0.02                | 0.28       |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 20                  | 0.28     | 0.0                 | 0.28       |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 20                  | 0.28     | 0.01                | 0.28       |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 20                  | 0.27     | 0.05                | 0.28       |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 20                  | 0.27     | 0.05                | 0.28       |
| (2,1136) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:H    | 20                  | 0.27     | 0.05                | 0.28       |
| (2,1155) | 2:1743:A:VAL:HG21 | 2:1744:A:HIS:H    | 20                  | 0.27     | 0.04                | 0.27       |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 20                  | 0.27     | 0.04                | 0.27       |
| (2,1155) | 2:1743:A:VAL:HG22 | 2:1744:A:HIS:H    | 20                  | 0.27     | 0.04                | 0.27       |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 20                  | 0.27     | 0.02                | 0.27       |
| (2,1034) | 2:1735:A:ILE:HG21 | 2:1739:A:ILE:HB   | 20                  | 0.27     | 0.02                | 0.27       |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 20                  | 0.27     | 0.02                | 0.27       |
| (2,960)  | 2:1739:A:ILE:HD13 | 2:1735:A:ILE:HG23 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG21 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG23 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG23 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG22 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG22 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG21 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,960)  | 2:1739:A:ILE:HD13 | 2:1735:A:ILE:HG22 | 20                  | 0.27     | 0.07                | 0.26       |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 20                  | 0.27     | 0.03                | 0.26       |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 20                  | 0.27     | 0.03                | 0.26       |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG21 | 20                  | 0.27     | 0.03                | 0.26       |
| (2,1175) | 2:1755:A:LEU:HD11 | 2:1755:A:LEU:HA   | 20                  | 0.27     | 0.05                | 0.3        |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 20                  | 0.27     | 0.05                | 0.3        |
| (2,1175) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:HA   | 20                  | 0.27     | 0.05                | 0.3        |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 20                  | 0.27     | 0.11                | 0.32       |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG23 | 20                  | 0.25     | 0.02                | 0.25       |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 20                  | 0.25     | 0.02                | 0.25       |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG22 | 20                  | 0.25     | 0.02                | 0.25       |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 20                  | 0.25     | 0.02                | 0.24       |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 20                  | 0.24     | 0.01                | 0.25       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 20                  | 0.24     | 0.01                | 0.24       |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 20                  | 0.24     | 0.01                | 0.24       |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 20                  | 0.24     | 0.05                | 0.24       |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 20                  | 0.23     | 0.01                | 0.23       |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 20                  | 0.23     | 0.01                | 0.23       |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 20                  | 0.23     | 0.04                | 0.22       |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 20                  | 0.22     | 0.01                | 0.22       |
| (2,1038) | 2:1735:A:ILE:HG21 | 2:1736:A:GLN:H    | 20                  | 0.22     | 0.01                | 0.22       |
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 20                  | 0.22     | 0.01                | 0.22       |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 20                  | 0.21     | 0.09                | 0.19       |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 20                  | 0.2      | 0.08                | 0.14       |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 20                  | 0.2      | 0.0                 | 0.2        |
| (2,22)   | 2:1809:A:ILE:HG21 | 2:1809:A:ILE:H    | 20                  | 0.19     | 0.02                | 0.19       |
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 20                  | 0.19     | 0.02                | 0.19       |
| (2,22)   | 2:1809:A:ILE:HG23 | 2:1809:A:ILE:H    | 20                  | 0.19     | 0.02                | 0.19       |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 20                  | 0.19     | 0.03                | 0.18       |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 20                  | 0.19     | 0.05                | 0.18       |
| (2,1376) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HA   | 20                  | 0.18     | 0.02                | 0.19       |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 20                  | 0.18     | 0.02                | 0.19       |
| (2,1376) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HA   | 20                  | 0.18     | 0.02                | 0.19       |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 20                  | 0.18     | 0.03                | 0.18       |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 20                  | 0.18     | 0.03                | 0.18       |
| (2,1428) | 2:1790:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 20                  | 0.18     | 0.03                | 0.18       |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 20                  | 0.18     | 0.03                | 0.18       |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 20                  | 0.18     | 0.03                | 0.18       |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 20                  | 0.18     | 0.03                | 0.18       |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD11 | 20                  | 0.18     | 0.03                | 0.18       |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG23 | 20                  | 0.17     | 0.02                | 0.17       |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 20                  | 0.17     | 0.02                | 0.17       |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG21 | 20                  | 0.17     | 0.02                | 0.17       |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 20                  | 0.17     | 0.03                | 0.16       |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 20                  | 0.17     | 0.03                | 0.16       |
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 20                  | 0.14     | 0.01                | 0.14       |
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG21  | 20                  | 0.14     | 0.01                | 0.14       |
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG22  | 20                  | 0.14     | 0.01                | 0.14       |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 20                  | 0.14     | 0.01                | 0.14       |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB3  | 20                  | 0.14     | 0.01                | 0.14       |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB2  | 20                  | 0.14     | 0.01                | 0.14       |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 20                  | 0.13     | 0.01                | 0.13       |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 19                  | 1.42     | 0.06                | 1.42       |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 19                  | 0.95     | 0.28                | 0.87       |
| (2,636)  | 1:135:B:LEU:HD21  | 1:132:B:GLU:HB2   | 19                  | 0.92     | 0.98                | 0.28       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,636)  | 1:135:B:LEU:HD22  | 1:132:B:GLU:HB2   | 19                  | 0.92     | 0.98                | 0.28       |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 19                  | 0.92     | 0.98                | 0.28       |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 19                  | 0.91     | 0.08                | 0.94       |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 19                  | 0.9      | 0.52                | 1.11       |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 19                  | 0.74     | 0.01                | 0.74       |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 19                  | 0.74     | 0.01                | 0.74       |
| (2,1452) | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:HB3  | 19                  | 0.74     | 0.01                | 0.74       |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 19                  | 0.72     | 0.06                | 0.75       |
| (2,1659) | 2:1809:A:ILE:HD11 | 2:1808:A:ASN:HB2  | 19                  | 0.69     | 0.06                | 0.71       |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 19                  | 0.69     | 0.06                | 0.71       |
| (2,1659) | 2:1809:A:ILE:HD12 | 2:1808:A:ASN:HB2  | 19                  | 0.69     | 0.06                | 0.71       |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD13  | 19                  | 0.65     | 0.26                | 0.51       |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 19                  | 0.65     | 0.26                | 0.51       |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD11  | 19                  | 0.65     | 0.26                | 0.51       |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 19                  | 0.58     | 0.21                | 0.68       |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 19                  | 0.57     | 0.13                | 0.55       |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG22  | 19                  | 0.57     | 0.13                | 0.55       |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG23  | 19                  | 0.57     | 0.13                | 0.55       |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD1  | 19                  | 0.52     | 0.23                | 0.61       |
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD1  | 19                  | 0.52     | 0.23                | 0.61       |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD2  | 19                  | 0.52     | 0.23                | 0.61       |
| (2,1451) | 2:1789:A:ALA:HB1  | 2:1805:A:PHE:HD2  | 19                  | 0.52     | 0.23                | 0.61       |
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD2  | 19                  | 0.52     | 0.23                | 0.61       |
| (2,1451) | 2:1789:A:ALA:HB1  | 2:1805:A:PHE:HD1  | 19                  | 0.52     | 0.23                | 0.61       |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD21 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD21 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD23 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD22 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HD22 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD22 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD23 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HD21 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,1083) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HD23 | 19                  | 0.49     | 0.2                 | 0.39       |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD12 | 19                  | 0.45     | 0.09                | 0.44       |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 19                  | 0.45     | 0.09                | 0.44       |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 19                  | 0.45     | 0.09                | 0.44       |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 19                  | 0.44     | 0.07                | 0.44       |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG22  | 19                  | 0.44     | 0.07                | 0.44       |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG23  | 19                  | 0.44     | 0.07                | 0.44       |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 19                  | 0.4      | 0.01                | 0.4        |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 19                  | 0.38     | 0.26                | 0.24       |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 19                  | 0.36     | 0.03                | 0.36       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 19                  | 0.36     | 0.03                | 0.36       |
| (2,997)  | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:H    | 19                  | 0.36     | 0.03                | 0.36       |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 19                  | 0.35     | 0.38                | 0.23       |
| (2,685)  | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG2  | 19                  | 0.29     | 0.09                | 0.32       |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 19                  | 0.29     | 0.09                | 0.32       |
| (2,685)  | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG2  | 19                  | 0.29     | 0.09                | 0.32       |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 19                  | 0.26     | 0.04                | 0.25       |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 19                  | 0.21     | 0.02                | 0.2        |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 19                  | 0.19     | 0.03                | 0.18       |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG21 | 19                  | 0.19     | 0.02                | 0.18       |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG23 | 19                  | 0.19     | 0.02                | 0.18       |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG22 | 19                  | 0.19     | 0.02                | 0.18       |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG22 | 19                  | 0.19     | 0.02                | 0.18       |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG23 | 19                  | 0.19     | 0.02                | 0.18       |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG21 | 19                  | 0.19     | 0.02                | 0.18       |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 19                  | 0.18     | 0.04                | 0.18       |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 19                  | 0.16     | 0.04                | 0.16       |
| (2,878)  | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 19                  | 0.16     | 0.05                | 0.14       |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD13 | 19                  | 0.16     | 0.03                | 0.16       |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 19                  | 0.16     | 0.03                | 0.16       |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD12 | 19                  | 0.16     | 0.03                | 0.16       |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 19                  | 0.14     | 0.01                | 0.14       |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD12 | 19                  | 0.14     | 0.01                | 0.14       |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD13 | 19                  | 0.14     | 0.01                | 0.14       |
| (2,717)  | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H    | 19                  | 0.14     | 0.01                | 0.14       |
| (2,717)  | 2:1790:A:ALA:HB2  | 2:1790:A:ALA:H    | 19                  | 0.14     | 0.01                | 0.14       |
| (2,717)  | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H    | 19                  | 0.14     | 0.01                | 0.14       |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD22 | 18                  | 2.03     | 0.37                | 2.08       |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD23 | 18                  | 2.03     | 0.37                | 2.08       |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD21 | 18                  | 2.03     | 0.37                | 2.08       |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 18                  | 0.98     | 0.59                | 1.35       |
| (2,1135) | 2:1765:A:VAL:HG12 | 2:1804:A:PRO:HG2  | 18                  | 0.98     | 0.59                | 1.35       |
| (2,1135) | 2:1765:A:VAL:HG11 | 2:1804:A:PRO:HG2  | 18                  | 0.98     | 0.59                | 1.35       |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 18                  | 0.84     | 0.07                | 0.8        |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 18                  | 0.66     | 0.13                | 0.68       |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 18                  | 0.56     | 0.25                | 0.66       |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 18                  | 0.49     | 0.04                | 0.48       |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 18                  | 0.46     | 0.38                | 0.18       |
| (2,1153) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HG2  | 18                  | 0.39     | 0.08                | 0.4        |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 18                  | 0.39     | 0.08                | 0.4        |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 18                  | 0.39     | 0.08                | 0.4        |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 18                  | 0.38     | 0.16                | 0.36       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1551) | 2:1735:A:ILE:HG22 | 2:1791:A:TYR:HB2  | 18                  | 0.38     | 0.16                | 0.36       |
| (2,1551) | 2:1735:A:ILE:HG23 | 2:1791:A:TYR:HB2  | 18                  | 0.38     | 0.16                | 0.36       |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 18                  | 0.35     | 0.44                | 0.21       |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 18                  | 0.31     | 0.05                | 0.3        |
| (2,1529) | 2:1746:A:ALA:HB3  | 2:1747:A:GLN:HG3  | 18                  | 0.31     | 0.05                | 0.3        |
| (2,1529) | 2:1746:A:ALA:HB2  | 2:1747:A:GLN:HG3  | 18                  | 0.31     | 0.05                | 0.3        |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 18                  | 0.27     | 0.1                 | 0.24       |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 18                  | 0.26     | 0.05                | 0.26       |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 18                  | 0.21     | 0.18                | 0.15       |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 18                  | 0.2      | 0.03                | 0.21       |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 18                  | 0.17     | 0.03                | 0.18       |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 18                  | 0.17     | 0.03                | 0.16       |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 18                  | 0.17     | 0.03                | 0.16       |
| (2,557)  | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD13  | 18                  | 0.12     | 0.0                 | 0.12       |
| (2,557)  | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD12  | 18                  | 0.12     | 0.0                 | 0.12       |
| (2,557)  | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD11  | 18                  | 0.12     | 0.0                 | 0.12       |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 17                  | 1.58     | 0.08                | 1.6        |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 17                  | 0.94     | 0.21                | 0.99       |
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 17                  | 0.66     | 0.14                | 0.63       |
| (2,465)  | 1:137:B:LEU:HD23  | 1:138:B:MET:H     | 17                  | 0.66     | 0.14                | 0.63       |
| (2,465)  | 1:137:B:LEU:HD21  | 1:138:B:MET:H     | 17                  | 0.66     | 0.14                | 0.63       |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG22  | 17                  | 0.57     | 0.12                | 0.56       |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 17                  | 0.57     | 0.12                | 0.56       |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG23  | 17                  | 0.57     | 0.12                | 0.56       |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 17                  | 0.47     | 0.0                 | 0.47       |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 17                  | 0.44     | 0.14                | 0.5        |
| (2,463)  | 1:134:B:ILE:HD12  | 1:134:B:ILE:H     | 17                  | 0.44     | 0.14                | 0.5        |
| (2,463)  | 1:134:B:ILE:HD11  | 1:134:B:ILE:H     | 17                  | 0.44     | 0.14                | 0.5        |
| (2,1150) | 2:1743:A:VAL:HG23 | 2:1803:A:VAL:HG11 | 17                  | 0.39     | 0.13                | 0.38       |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG12 | 17                  | 0.39     | 0.13                | 0.38       |
| (2,1150) | 2:1743:A:VAL:HG21 | 2:1803:A:VAL:HG12 | 17                  | 0.39     | 0.13                | 0.38       |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG11 | 17                  | 0.39     | 0.13                | 0.38       |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG13 | 17                  | 0.39     | 0.13                | 0.38       |
| (2,1150) | 2:1743:A:VAL:HG23 | 2:1803:A:VAL:HG13 | 17                  | 0.39     | 0.13                | 0.38       |
| (2,1150) | 2:1743:A:VAL:HG23 | 2:1803:A:VAL:HG12 | 17                  | 0.39     | 0.13                | 0.38       |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 17                  | 0.35     | 0.09                | 0.38       |
| (2,576)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:H     | 17                  | 0.19     | 0.06                | 0.19       |
| (2,576)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:H     | 17                  | 0.19     | 0.06                | 0.19       |
| (2,576)  | 1:119:B:VAL:HG11  | 1:120:B:ILE:H     | 17                  | 0.19     | 0.06                | 0.19       |
| (2,914)  | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 17                  | 0.15     | 0.06                | 0.14       |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 17                  | 0.14     | 0.02                | 0.14       |
| (2,917)  | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H    | 17                  | 0.13     | 0.02                | 0.11       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 16                  | 0.52     | 0.18                | 0.57       |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 16                  | 0.52     | 0.18                | 0.57       |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD11  | 16                  | 0.52     | 0.18                | 0.57       |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 16                  | 0.35     | 0.44                | 0.17       |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 16                  | 0.33     | 0.03                | 0.33       |
| (2,540)  | 1:134:B:ILE:HG21  | 2:1781:A:ILE:HA   | 16                  | 0.28     | 0.09                | 0.25       |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 16                  | 0.28     | 0.09                | 0.25       |
| (2,540)  | 1:134:B:ILE:HG22  | 2:1781:A:ILE:HA   | 16                  | 0.28     | 0.09                | 0.25       |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB1  | 16                  | 0.2      | 0.08                | 0.19       |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 16                  | 0.2      | 0.08                | 0.19       |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB2  | 16                  | 0.2      | 0.08                | 0.19       |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 16                  | 0.2      | 0.07                | 0.19       |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG22  | 16                  | 0.2      | 0.07                | 0.19       |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG21  | 16                  | 0.2      | 0.07                | 0.19       |
| (2,1506) | 2:1781:A:ILE:HD11 | 2:1781:A:ILE:H    | 16                  | 0.2      | 0.07                | 0.2        |
| (2,1506) | 2:1781:A:ILE:HD12 | 2:1781:A:ILE:H    | 16                  | 0.2      | 0.07                | 0.2        |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 16                  | 0.2      | 0.07                | 0.2        |
| (2,1397) | 2:1793:A:ALA:HB2  | 2:1794:A:LYS:H    | 16                  | 0.18     | 0.05                | 0.16       |
| (2,1397) | 2:1793:A:ALA:HB1  | 2:1794:A:LYS:H    | 16                  | 0.18     | 0.05                | 0.16       |
| (2,1397) | 2:1793:A:ALA:HB3  | 2:1794:A:LYS:H    | 16                  | 0.18     | 0.05                | 0.16       |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 16                  | 0.14     | 0.03                | 0.15       |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 15                  | 1.12     | 0.09                | 1.14       |
| (2,850)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB3  | 15                  | 1.1      | 0.56                | 1.28       |
| (2,850)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB3  | 15                  | 1.1      | 0.56                | 1.28       |
| (2,850)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB3  | 15                  | 1.1      | 0.56                | 1.28       |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 15                  | 0.78     | 0.07                | 0.76       |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 15                  | 0.68     | 0.34                | 0.94       |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD11 | 15                  | 0.59     | 0.3                 | 0.51       |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD12 | 15                  | 0.59     | 0.3                 | 0.51       |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD13 | 15                  | 0.59     | 0.3                 | 0.51       |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 15                  | 0.51     | 0.21                | 0.52       |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 15                  | 0.45     | 0.0                 | 0.45       |
| (2,634)  | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 15                  | 0.4      | 0.01                | 0.4        |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 15                  | 0.35     | 0.11                | 0.37       |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB3  | 15                  | 0.26     | 0.09                | 0.24       |
| (2,923)  | 2:1765:A:VAL:HG23 | 2:1745:A:ALA:HB3  | 15                  | 0.26     | 0.09                | 0.24       |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB1  | 15                  | 0.26     | 0.09                | 0.24       |
| (2,923)  | 2:1765:A:VAL:HG23 | 2:1745:A:ALA:HB1  | 15                  | 0.26     | 0.09                | 0.24       |
| (2,923)  | 2:1765:A:VAL:HG21 | 2:1745:A:ALA:HB1  | 15                  | 0.26     | 0.09                | 0.24       |
| (2,923)  | 2:1765:A:VAL:HG21 | 2:1745:A:ALA:HB2  | 15                  | 0.26     | 0.09                | 0.24       |
| (2,923)  | 2:1765:A:VAL:HG21 | 2:1745:A:ALA:HB3  | 15                  | 0.26     | 0.09                | 0.24       |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB2  | 15                  | 0.26     | 0.09                | 0.24       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 15                  | 0.24     | 0.02                | 0.23       |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD12 | 15                  | 0.2      | 0.05                | 0.2        |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD13 | 15                  | 0.2      | 0.05                | 0.2        |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD11 | 15                  | 0.2      | 0.05                | 0.2        |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 15                  | 0.2      | 0.06                | 0.19       |
| (2,1530) | 2:1746:A:ALA:HB3  | 2:1802:A:PRO:HB2  | 15                  | 0.2      | 0.06                | 0.19       |
| (2,1530) | 2:1746:A:ALA:HB2  | 2:1802:A:PRO:HB2  | 15                  | 0.2      | 0.06                | 0.19       |
| (3,36)   | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG3  | 15                  | 0.17     | 0.05                | 0.16       |
| (3,36)   | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG3  | 15                  | 0.17     | 0.05                | 0.16       |
| (3,36)   | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG3  | 15                  | 0.17     | 0.05                | 0.16       |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 15                  | 0.13     | 0.02                | 0.13       |
| (2,846)  | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB3  | 15                  | 0.13     | 0.02                | 0.12       |
| (2,846)  | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1  | 15                  | 0.13     | 0.02                | 0.12       |
| (2,846)  | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB2  | 15                  | 0.13     | 0.02                | 0.12       |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 15                  | 0.12     | 0.01                | 0.12       |
| (2,1383) | 2:1785:A:LEU:HD12 | 2:1785:A:LEU:HA   | 14                  | 1.27     | 0.59                | 1.56       |
| (2,1383) | 2:1785:A:LEU:HD11 | 2:1785:A:LEU:HA   | 14                  | 1.27     | 0.59                | 1.56       |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 14                  | 1.27     | 0.59                | 1.56       |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 14                  | 1.2      | 0.45                | 1.22       |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 14                  | 1.06     | 0.41                | 0.9        |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 14                  | 0.72     | 0.01                | 0.72       |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 14                  | 0.72     | 0.43                | 0.91       |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 14                  | 0.56     | 0.03                | 0.56       |
| (2,484)  | 1:126:B:LEU:HD13  | 1:126:B:LEU:HA    | 14                  | 0.56     | 0.03                | 0.56       |
| (2,484)  | 1:126:B:LEU:HD12  | 1:126:B:LEU:HA    | 14                  | 0.56     | 0.03                | 0.56       |
| (2,1699) | 2:1781:A:ILE:HD12 | 2:1767:A:HIS:HD2  | 14                  | 0.41     | 0.11                | 0.44       |
| (2,1699) | 2:1781:A:ILE:HD13 | 2:1767:A:HIS:HD2  | 14                  | 0.41     | 0.11                | 0.44       |
| (2,1699) | 2:1781:A:ILE:HD11 | 2:1767:A:HIS:HD2  | 14                  | 0.41     | 0.11                | 0.44       |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 14                  | 0.37     | 0.11                | 0.36       |
| (2,1156) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HE22 | 14                  | 0.37     | 0.11                | 0.36       |
| (2,1156) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HE22 | 14                  | 0.37     | 0.11                | 0.36       |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 14                  | 0.25     | 0.08                | 0.25       |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG13 | 14                  | 0.22     | 0.05                | 0.24       |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG12 | 14                  | 0.22     | 0.05                | 0.24       |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG11 | 14                  | 0.22     | 0.05                | 0.24       |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 14                  | 0.17     | 0.05                | 0.17       |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 14                  | 0.15     | 0.03                | 0.15       |
| (3,9)    | 1:120:B:ILE:HG22  | 1:120:B:ILE:HG12  | 14                  | 0.14     | 0.02                | 0.14       |
| (3,9)    | 1:120:B:ILE:HG21  | 1:120:B:ILE:HG12  | 14                  | 0.14     | 0.02                | 0.14       |
| (3,9)    | 1:120:B:ILE:HG23  | 1:120:B:ILE:HG12  | 14                  | 0.14     | 0.02                | 0.14       |
| (2,906)  | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 13                  | 1.71     | 0.66                | 2.1        |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 13                  | 1.52     | 0.14                | 1.58       |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 13                  | 1.43     | 0.11                | 1.42       |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD22 | 13                  | 1.27     | 0.16                | 1.31       |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD23 | 13                  | 1.27     | 0.16                | 1.31       |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD21 | 13                  | 1.27     | 0.16                | 1.31       |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD23 | 13                  | 1.19     | 0.39                | 1.31       |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD21 | 13                  | 1.19     | 0.39                | 1.31       |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD22 | 13                  | 1.19     | 0.39                | 1.31       |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 13                  | 1.09     | 0.11                | 1.1        |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 13                  | 0.93     | 0.67                | 0.65       |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 13                  | 0.68     | 0.14                | 0.65       |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 13                  | 0.68     | 0.3                 | 0.88       |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 13                  | 0.61     | 0.25                | 0.53       |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 13                  | 0.58     | 0.3                 | 0.69       |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 13                  | 0.58     | 0.3                 | 0.52       |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 13                  | 0.4      | 0.03                | 0.41       |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 13                  | 0.32     | 0.01                | 0.32       |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 13                  | 0.24     | 0.11                | 0.19       |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD2   | 13                  | 0.24     | 0.11                | 0.19       |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 13                  | 0.14     | 0.01                | 0.14       |
| (2,1654) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HG3  | 12                  | 1.43     | 0.39                | 1.52       |
| (2,1654) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HG3  | 12                  | 1.43     | 0.39                | 1.52       |
| (2,1654) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HG3  | 12                  | 1.43     | 0.39                | 1.52       |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD22 | 12                  | 1.42     | 0.01                | 1.42       |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD23 | 12                  | 1.42     | 0.01                | 1.42       |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD21 | 12                  | 1.42     | 0.01                | 1.42       |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 12                  | 1.15     | 0.1                 | 1.13       |
| (2,851)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB2  | 12                  | 1.03     | 0.33                | 0.88       |
| (2,851)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB2  | 12                  | 1.03     | 0.33                | 0.88       |
| (2,851)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB2  | 12                  | 1.03     | 0.33                | 0.88       |
| (2,853)  | 2:1807:A:LEU:HD23 | 2:1807:A:LEU:H    | 12                  | 0.75     | 0.05                | 0.76       |
| (2,853)  | 2:1807:A:LEU:HD21 | 2:1807:A:LEU:H    | 12                  | 0.75     | 0.05                | 0.76       |
| (2,853)  | 2:1807:A:LEU:HD22 | 2:1807:A:LEU:H    | 12                  | 0.75     | 0.05                | 0.76       |
| (2,1344) | 2:1755:A:LEU:HD22 | 2:1756:A:PRO:HD3  | 12                  | 0.53     | 0.02                | 0.54       |
| (2,1344) | 2:1755:A:LEU:HD23 | 2:1756:A:PRO:HD3  | 12                  | 0.53     | 0.02                | 0.54       |
| (2,1344) | 2:1755:A:LEU:HD21 | 2:1756:A:PRO:HD3  | 12                  | 0.53     | 0.02                | 0.54       |
| (2,1244) | 2:1775:A:THR:HG22 | 2:1776:A:ASN:HB2  | 12                  | 0.41     | 0.13                | 0.4        |
| (2,1244) | 2:1775:A:THR:HG23 | 2:1776:A:ASN:HB2  | 12                  | 0.41     | 0.13                | 0.4        |
| (2,1244) | 2:1775:A:THR:HG21 | 2:1776:A:ASN:HB2  | 12                  | 0.41     | 0.13                | 0.4        |
| (2,1346) | 2:1755:A:LEU:HD23 | 2:1758:A:CYS:HB3  | 12                  | 0.38     | 0.08                | 0.34       |
| (2,1346) | 2:1755:A:LEU:HD21 | 2:1758:A:CYS:HB3  | 12                  | 0.38     | 0.08                | 0.34       |
| (2,1346) | 2:1755:A:LEU:HD22 | 2:1758:A:CYS:HB3  | 12                  | 0.38     | 0.08                | 0.34       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1146) | 2:1788:A:LEU:HD23 | 2:1735:A:ILE:HA   | 12                  | 0.29     | 0.15                | 0.23       |
| (2,1146) | 2:1788:A:LEU:HD21 | 2:1735:A:ILE:HA   | 12                  | 0.29     | 0.15                | 0.23       |
| (2,1146) | 2:1788:A:LEU:HD22 | 2:1735:A:ILE:HA   | 12                  | 0.29     | 0.15                | 0.23       |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 12                  | 0.28     | 0.09                | 0.25       |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1   | 12                  | 0.26     | 0.13                | 0.22       |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE2   | 12                  | 0.26     | 0.13                | 0.22       |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 12                  | 0.2      | 0.05                | 0.21       |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 12                  | 0.15     | 0.03                | 0.16       |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 12                  | 0.13     | 0.02                | 0.13       |
| (3,30)   | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HD2  | 12                  | 0.11     | 0.01                | 0.11       |
| (3,30)   | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HB2  | 12                  | 0.11     | 0.01                | 0.11       |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 11                  | 1.17     | 0.56                | 1.48       |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 11                  | 0.45     | 0.08                | 0.47       |
| (2,617)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:HA    | 11                  | 0.38     | 0.12                | 0.34       |
| (2,617)  | 1:137:B:LEU:HD21  | 1:137:B:LEU:HA    | 11                  | 0.38     | 0.12                | 0.34       |
| (2,617)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:HA    | 11                  | 0.38     | 0.12                | 0.34       |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 11                  | 0.32     | 0.03                | 0.33       |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 11                  | 0.31     | 0.01                | 0.31       |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 11                  | 0.28     | 0.07                | 0.28       |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG23 | 11                  | 0.27     | 0.03                | 0.26       |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG22 | 11                  | 0.27     | 0.03                | 0.26       |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG21 | 11                  | 0.27     | 0.03                | 0.26       |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 11                  | 0.27     | 0.19                | 0.19       |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 11                  | 0.25     | 0.02                | 0.25       |
| (2,114)  | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 11                  | 0.17     | 0.04                | 0.17       |
| (2,1014) | 2:1733:A:LEU:HD23 | 2:1733:A:LEU:H    | 11                  | 0.15     | 0.04                | 0.14       |
| (2,1014) | 2:1733:A:LEU:HD22 | 2:1733:A:LEU:H    | 11                  | 0.15     | 0.04                | 0.14       |
| (2,1014) | 2:1733:A:LEU:HD21 | 2:1733:A:LEU:H    | 11                  | 0.15     | 0.04                | 0.14       |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 11                  | 0.14     | 0.03                | 0.13       |
| (2,1293) | 2:1745:A:ALA:HB3  | 2:1746:A:ALA:H    | 11                  | 0.14     | 0.02                | 0.14       |
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 11                  | 0.14     | 0.02                | 0.14       |
| (2,1293) | 2:1745:A:ALA:HB2  | 2:1746:A:ALA:H    | 11                  | 0.14     | 0.02                | 0.14       |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 11                  | 0.12     | 0.03                | 0.12       |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 11                  | 0.12     | 0.01                | 0.12       |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE2   | 10                  | 1.61     | 0.11                | 1.63       |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 10                  | 1.61     | 0.11                | 1.63       |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 10                  | 1.14     | 0.09                | 1.12       |
| (2,487)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 10                  | 0.71     | 0.71                | 0.14       |
| (2,464)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:H     | 10                  | 0.56     | 0.11                | 0.6        |
| (2,464)  | 1:137:B:LEU:HD21  | 1:137:B:LEU:H     | 10                  | 0.56     | 0.11                | 0.6        |
| (2,464)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:H     | 10                  | 0.56     | 0.11                | 0.6        |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 10                  | 0.5      | 0.0                 | 0.5        |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,669)  | 1:120:B:ILE:HG21  | 1:117:B:ASP:H     | 10                  | 0.44     | 0.16                | 0.47       |
| (2,669)  | 1:120:B:ILE:HG22  | 1:117:B:ASP:H     | 10                  | 0.44     | 0.16                | 0.47       |
| (2,669)  | 1:120:B:ILE:HG23  | 1:117:B:ASP:H     | 10                  | 0.44     | 0.16                | 0.47       |
| (2,661)  | 1:111:B:ALA:HB1   | 1:112:B:SER:HB3   | 10                  | 0.43     | 0.13                | 0.42       |
| (2,661)  | 1:111:B:ALA:HB3   | 1:112:B:SER:HB3   | 10                  | 0.43     | 0.13                | 0.42       |
| (2,661)  | 1:111:B:ALA:HB2   | 1:112:B:SER:HB3   | 10                  | 0.43     | 0.13                | 0.42       |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD23 | 10                  | 0.42     | 0.12                | 0.41       |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD22 | 10                  | 0.42     | 0.12                | 0.41       |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD21 | 10                  | 0.42     | 0.12                | 0.41       |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD23 | 10                  | 0.42     | 0.12                | 0.41       |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD21 | 10                  | 0.42     | 0.12                | 0.41       |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD22 | 10                  | 0.42     | 0.12                | 0.41       |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 10                  | 0.37     | 0.02                | 0.37       |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 10                  | 0.36     | 0.14                | 0.32       |
| (2,247)  | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 10                  | 0.2      | 0.09                | 0.18       |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE1   | 10                  | 0.18     | 0.03                | 0.18       |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE2   | 10                  | 0.18     | 0.03                | 0.18       |
| (2,1570) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HE1   | 10                  | 0.18     | 0.03                | 0.18       |
| (2,1570) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HE2   | 10                  | 0.18     | 0.03                | 0.18       |
| (1,35)   | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 10                  | 0.15     | 0.03                | 0.16       |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 10                  | 0.15     | 0.02                | 0.16       |
| (2,108)  | 2:1741:A:SER:H    | 2:1761:A:MET:HE1  | 10                  | 0.13     | 0.03                | 0.12       |
| (2,108)  | 2:1741:A:SER:H    | 2:1761:A:MET:HE2  | 10                  | 0.13     | 0.03                | 0.12       |
| (2,108)  | 2:1741:A:SER:H    | 2:1761:A:MET:HE3  | 10                  | 0.13     | 0.03                | 0.12       |
| (2,666)  | 1:120:B:ILE:HD12  | 1:117:B:ASP:HB3   | 9                   | 0.74     | 0.48                | 0.6        |
| (2,666)  | 1:120:B:ILE:HD11  | 1:117:B:ASP:HB3   | 9                   | 0.74     | 0.48                | 0.6        |
| (2,666)  | 1:120:B:ILE:HD13  | 1:117:B:ASP:HB3   | 9                   | 0.74     | 0.48                | 0.6        |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 9                   | 0.61     | 0.01                | 0.61       |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 9                   | 0.59     | 0.02                | 0.59       |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 9                   | 0.58     | 0.0                 | 0.58       |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 9                   | 0.52     | 0.22                | 0.65       |
| (2,1385) | 2:1785:A:LEU:HD11 | 2:1768:A:THR:HG23 | 9                   | 0.45     | 0.14                | 0.49       |
| (2,1385) | 2:1785:A:LEU:HD11 | 2:1768:A:THR:HG21 | 9                   | 0.45     | 0.14                | 0.49       |
| (2,1385) | 2:1785:A:LEU:HD13 | 2:1768:A:THR:HG22 | 9                   | 0.45     | 0.14                | 0.49       |
| (2,1385) | 2:1785:A:LEU:HD13 | 2:1768:A:THR:HG21 | 9                   | 0.45     | 0.14                | 0.49       |
| (2,1385) | 2:1785:A:LEU:HD11 | 2:1768:A:THR:HG22 | 9                   | 0.45     | 0.14                | 0.49       |
| (2,1385) | 2:1785:A:LEU:HD12 | 2:1768:A:THR:HG23 | 9                   | 0.45     | 0.14                | 0.49       |
| (2,1385) | 2:1785:A:LEU:HD12 | 2:1768:A:THR:HG21 | 9                   | 0.45     | 0.14                | 0.49       |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 9                   | 0.4      | 0.14                | 0.37       |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 9                   | 0.39     | 0.01                | 0.39       |
| (2,1081) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HG   | 9                   | 0.37     | 0.03                | 0.36       |
| (2,1081) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HG   | 9                   | 0.37     | 0.03                | 0.36       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1081) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HG   | 9                   | 0.37     | 0.03                | 0.36       |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 9                   | 0.37     | 0.12                | 0.38       |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD2  | 9                   | 0.37     | 0.12                | 0.38       |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG23  | 9                   | 0.34     | 0.17                | 0.27       |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG22  | 9                   | 0.34     | 0.17                | 0.27       |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG21  | 9                   | 0.34     | 0.17                | 0.27       |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG23  | 9                   | 0.33     | 0.14                | 0.34       |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG21  | 9                   | 0.33     | 0.14                | 0.34       |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG22  | 9                   | 0.33     | 0.14                | 0.34       |
| (2,1737) | 2:1785:A:LEU:HD11 | 2:1767:A:HIS:HD2  | 9                   | 0.31     | 0.09                | 0.29       |
| (2,1737) | 2:1785:A:LEU:HD13 | 2:1767:A:HIS:HD2  | 9                   | 0.31     | 0.09                | 0.29       |
| (2,1737) | 2:1785:A:LEU:HD12 | 2:1767:A:HIS:HD2  | 9                   | 0.31     | 0.09                | 0.29       |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 9                   | 0.29     | 0.04                | 0.3        |
| (2,1387) | 2:1785:A:LEU:HD11 | 2:1805:A:PHE:HE1  | 9                   | 0.28     | 0.05                | 0.26       |
| (2,1387) | 2:1785:A:LEU:HD13 | 2:1805:A:PHE:HE2  | 9                   | 0.28     | 0.05                | 0.26       |
| (2,1387) | 2:1785:A:LEU:HD11 | 2:1805:A:PHE:HE2  | 9                   | 0.28     | 0.05                | 0.26       |
| (2,1387) | 2:1785:A:LEU:HD12 | 2:1805:A:PHE:HE1  | 9                   | 0.28     | 0.05                | 0.26       |
| (2,1387) | 2:1785:A:LEU:HD12 | 2:1805:A:PHE:HE2  | 9                   | 0.28     | 0.05                | 0.26       |
| (2,1387) | 2:1785:A:LEU:HD13 | 2:1805:A:PHE:HE1  | 9                   | 0.28     | 0.05                | 0.26       |
| (2,1727) | 2:1781:A:ILE:HG23 | 2:1767:A:HIS:HD2  | 9                   | 0.27     | 0.06                | 0.26       |
| (2,1727) | 2:1781:A:ILE:HG22 | 2:1767:A:HIS:HD2  | 9                   | 0.27     | 0.06                | 0.26       |
| (2,1727) | 2:1781:A:ILE:HG21 | 2:1767:A:HIS:HD2  | 9                   | 0.27     | 0.06                | 0.26       |
| (2,903)  | 2:1768:A:THR:HA   | 2:1771:A:CYS:H    | 9                   | 0.13     | 0.02                | 0.14       |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD11  | 8                   | 1.89     | 1.02                | 1.69       |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD13  | 8                   | 1.89     | 1.02                | 1.69       |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD12  | 8                   | 1.89     | 1.02                | 1.69       |
| (2,524)  | 1:137:B:LEU:HD12  | 1:137:B:LEU:HB2   | 8                   | 1.04     | 0.31                | 1.16       |
| (2,524)  | 1:137:B:LEU:HD11  | 1:137:B:LEU:HB2   | 8                   | 1.04     | 0.31                | 1.16       |
| (2,524)  | 1:137:B:LEU:HD13  | 1:137:B:LEU:HB2   | 8                   | 1.04     | 0.31                | 1.16       |
| (2,1736) | 2:1755:A:LEU:HD13 | 2:1744:A:HIS:HD2  | 8                   | 0.67     | 0.02                | 0.67       |
| (2,1736) | 2:1755:A:LEU:HD12 | 2:1744:A:HIS:HD2  | 8                   | 0.67     | 0.02                | 0.67       |
| (2,1736) | 2:1755:A:LEU:HD11 | 2:1744:A:HIS:HD2  | 8                   | 0.67     | 0.02                | 0.67       |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 8                   | 0.65     | 0.02                | 0.65       |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 8                   | 0.59     | 0.34                | 0.73       |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 8                   | 0.57     | 0.24                | 0.56       |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 8                   | 0.55     | 0.06                | 0.52       |
| (2,1700) | 2:1755:A:LEU:HD11 | 2:1756:A:PRO:HG2  | 8                   | 0.54     | 0.03                | 0.54       |
| (2,1700) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HG2  | 8                   | 0.54     | 0.03                | 0.54       |
| (2,1700) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HG2  | 8                   | 0.54     | 0.03                | 0.54       |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD22 | 8                   | 0.53     | 0.01                | 0.53       |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD21 | 8                   | 0.53     | 0.01                | 0.53       |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD23 | 8                   | 0.53     | 0.01                | 0.53       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 8                   | 0.52     | 0.0                 | 0.52       |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG23 | 8                   | 0.47     | 0.03                | 0.46       |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG22 | 8                   | 0.47     | 0.03                | 0.46       |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG21 | 8                   | 0.47     | 0.03                | 0.46       |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 8                   | 0.47     | 0.01                | 0.47       |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 8                   | 0.42     | 0.19                | 0.37       |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 8                   | 0.39     | 0.14                | 0.36       |
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG23 | 8                   | 0.36     | 0.18                | 0.32       |
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG22 | 8                   | 0.36     | 0.18                | 0.32       |
| (2,1514) | 2:1764:A:VAL:HG12 | 2:1781:A:ILE:HG22 | 8                   | 0.36     | 0.18                | 0.32       |
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG21 | 8                   | 0.36     | 0.18                | 0.32       |
| (2,1514) | 2:1764:A:VAL:HG13 | 2:1781:A:ILE:HG22 | 8                   | 0.36     | 0.18                | 0.32       |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 8                   | 0.33     | 0.02                | 0.34       |
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 8                   | 0.3      | 0.18                | 0.26       |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG22  | 8                   | 0.2      | 0.08                | 0.18       |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG23  | 8                   | 0.2      | 0.08                | 0.18       |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG21  | 8                   | 0.2      | 0.08                | 0.18       |
| (2,455)  | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 8                   | 0.2      | 0.19                | 0.11       |
| (2,1371) | 2:1764:A:VAL:HG23 | 2:1764:A:VAL:H    | 8                   | 0.16     | 0.05                | 0.15       |
| (2,1371) | 2:1764:A:VAL:HG22 | 2:1764:A:VAL:H    | 8                   | 0.16     | 0.05                | 0.15       |
| (2,1371) | 2:1764:A:VAL:HG21 | 2:1764:A:VAL:H    | 8                   | 0.16     | 0.05                | 0.15       |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 8                   | 0.16     | 0.03                | 0.17       |
| (2,882)  | 2:1807:A:LEU:HG   | 2:1807:A:LEU:H    | 8                   | 0.15     | 0.08                | 0.12       |
| (2,483)  | 1:126:B:LEU:HD21  | 1:127:B:GLU:H     | 8                   | 0.13     | 0.02                | 0.14       |
| (2,483)  | 1:126:B:LEU:HD22  | 1:127:B:GLU:H     | 8                   | 0.13     | 0.02                | 0.14       |
| (2,483)  | 1:126:B:LEU:HD23  | 1:127:B:GLU:H     | 8                   | 0.13     | 0.02                | 0.14       |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA    | 7                   | 1.01     | 0.06                | 1.03       |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H    | 7                   | 0.97     | 0.04                | 0.98       |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 7                   | 0.63     | 0.0                 | 0.63       |
| (2,763)  | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 7                   | 0.54     | 0.19                | 0.61       |
| (2,1030) | 2:1807:A:LEU:HD12 | 2:1801:A:CYS:HB2  | 7                   | 0.51     | 0.24                | 0.34       |
| (2,1030) | 2:1807:A:LEU:HD11 | 2:1801:A:CYS:HB2  | 7                   | 0.51     | 0.24                | 0.34       |
| (2,1030) | 2:1807:A:LEU:HD13 | 2:1801:A:CYS:HB2  | 7                   | 0.51     | 0.24                | 0.34       |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD21 | 7                   | 0.45     | 0.06                | 0.43       |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD23 | 7                   | 0.45     | 0.06                | 0.43       |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD22  | 7                   | 0.38     | 0.03                | 0.39       |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD21  | 7                   | 0.38     | 0.03                | 0.39       |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD23  | 7                   | 0.38     | 0.03                | 0.39       |
| (2,522)  | 1:135:B:LEU:HD13  | 1:135:B:LEU:HA    | 7                   | 0.37     | 0.49                | 0.18       |
| (2,522)  | 1:135:B:LEU:HD11  | 1:135:B:LEU:HA    | 7                   | 0.37     | 0.49                | 0.18       |
| (2,522)  | 1:135:B:LEU:HD12  | 1:135:B:LEU:HA    | 7                   | 0.37     | 0.49                | 0.18       |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE2  | 7                   | 0.34     | 0.14                | 0.3        |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE1  | 7                   | 0.34     | 0.14                | 0.3        |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 7                   | 0.29     | 0.01                | 0.28       |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 7                   | 0.26     | 0.08                | 0.27       |
| (2,1379) | 2:1809:A:ILE:HG21 | 2:1793:A:ALA:HB2  | 7                   | 0.24     | 0.07                | 0.24       |
| (2,1379) | 2:1809:A:ILE:HG23 | 2:1793:A:ALA:HB2  | 7                   | 0.24     | 0.07                | 0.24       |
| (2,1379) | 2:1809:A:ILE:HG23 | 2:1793:A:ALA:HB1  | 7                   | 0.24     | 0.07                | 0.24       |
| (2,1379) | 2:1809:A:ILE:HG23 | 2:1793:A:ALA:HB3  | 7                   | 0.24     | 0.07                | 0.24       |
| (2,1379) | 2:1809:A:ILE:HG22 | 2:1793:A:ALA:HB1  | 7                   | 0.24     | 0.07                | 0.24       |
| (2,1127) | 2:1761:A:MET:HE3  | 2:1738:A:ALA:HB3  | 7                   | 0.19     | 0.05                | 0.22       |
| (2,1127) | 2:1761:A:MET:HE1  | 2:1738:A:ALA:HB3  | 7                   | 0.19     | 0.05                | 0.22       |
| (2,1127) | 2:1761:A:MET:HE2  | 2:1738:A:ALA:HB3  | 7                   | 0.19     | 0.05                | 0.22       |
| (2,1127) | 2:1761:A:MET:HE2  | 2:1738:A:ALA:HB1  | 7                   | 0.19     | 0.05                | 0.22       |
| (2,1127) | 2:1761:A:MET:HE1  | 2:1738:A:ALA:HB1  | 7                   | 0.19     | 0.05                | 0.22       |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 7                   | 0.19     | 0.0                 | 0.19       |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 7                   | 0.18     | 0.03                | 0.2        |
| (2,1119) | 2:1739:A:ILE:HG21 | 2:1736:A:GLN:HA   | 7                   | 0.17     | 0.04                | 0.14       |
| (2,1119) | 2:1739:A:ILE:HG22 | 2:1736:A:GLN:HA   | 7                   | 0.17     | 0.04                | 0.14       |
| (2,1119) | 2:1739:A:ILE:HG23 | 2:1736:A:GLN:HA   | 7                   | 0.17     | 0.04                | 0.14       |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 7                   | 0.16     | 0.01                | 0.16       |
| (2,543)  | 1:134:B:ILE:HG12  | 1:134:B:ILE:HA    | 7                   | 0.15     | 0.01                | 0.15       |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 7                   | 0.13     | 0.02                | 0.13       |
| (2,513)  | 1:126:B:LEU:HD11  | 1:123:B:ILE:HA    | 6                   | 1.54     | 0.65                | 1.82       |
| (2,513)  | 1:126:B:LEU:HD12  | 1:123:B:ILE:HA    | 6                   | 1.54     | 0.65                | 1.82       |
| (2,513)  | 1:126:B:LEU:HD13  | 1:123:B:ILE:HA    | 6                   | 1.54     | 0.65                | 1.82       |
| (2,676)  | 1:132:B:GLU:HG2   | 1:135:B:LEU:HB2   | 6                   | 1.0      | 0.34                | 1.09       |
| (2,1704) | 2:1801:A:CYS:HB2  | 2:1807:A:LEU:H    | 6                   | 0.89     | 0.17                | 0.82       |
| (2,679)  | 1:135:B:LEU:HD11  | 1:132:B:GLU:HA    | 6                   | 0.87     | 0.23                | 1.0        |
| (2,679)  | 1:135:B:LEU:HD12  | 1:132:B:GLU:HA    | 6                   | 0.87     | 0.23                | 1.0        |
| (2,679)  | 1:135:B:LEU:HD13  | 1:132:B:GLU:HA    | 6                   | 0.87     | 0.23                | 1.0        |
| (2,657)  | 1:135:B:LEU:HD22  | 1:130:B:TYR:HD2   | 6                   | 0.73     | 0.97                | 0.25       |
| (2,657)  | 1:135:B:LEU:HD21  | 1:130:B:TYR:HD1   | 6                   | 0.73     | 0.97                | 0.25       |
| (2,657)  | 1:135:B:LEU:HD22  | 1:130:B:TYR:HD1   | 6                   | 0.73     | 0.97                | 0.25       |
| (2,657)  | 1:135:B:LEU:HD23  | 1:130:B:TYR:HD2   | 6                   | 0.73     | 0.97                | 0.25       |
| (2,657)  | 1:135:B:LEU:HD23  | 1:130:B:TYR:HD1   | 6                   | 0.73     | 0.97                | 0.25       |
| (2,579)  | 1:126:B:LEU:HD23  | 1:126:B:LEU:HB3   | 6                   | 0.61     | 0.01                | 0.6        |
| (2,579)  | 1:126:B:LEU:HD22  | 1:126:B:LEU:HB3   | 6                   | 0.61     | 0.01                | 0.6        |
| (2,579)  | 1:126:B:LEU:HD21  | 1:126:B:LEU:HB3   | 6                   | 0.61     | 0.01                | 0.6        |
| (2,893)  | 2:1800:A:LYS:HG2  | 2:1800:A:LYS:HA   | 6                   | 0.58     | 0.02                | 0.58       |
| (2,819)  | 2:1749:A:ARG:HA   | 2:1749:A:ARG:HD3  | 6                   | 0.5      | 0.04                | 0.5        |
| (2,538)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HB2   | 6                   | 0.44     | 0.03                | 0.44       |
| (2,538)  | 1:126:B:LEU:HD12  | 1:126:B:LEU:HB2   | 6                   | 0.44     | 0.03                | 0.44       |
| (2,538)  | 1:126:B:LEU:HD13  | 1:126:B:LEU:HB2   | 6                   | 0.44     | 0.03                | 0.44       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1555) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HD1   | 6                   | 0.38     | 0.12                | 0.38       |
| (2,1555) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HD1   | 6                   | 0.38     | 0.12                | 0.38       |
| (2,1555) | 2:1735:A:ILE:HD13 | 1:130:B:TYR:HD2   | 6                   | 0.38     | 0.12                | 0.38       |
| (2,1555) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HD2   | 6                   | 0.38     | 0.12                | 0.38       |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG21  | 6                   | 0.3      | 0.13                | 0.3        |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG23  | 6                   | 0.3      | 0.13                | 0.3        |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG22  | 6                   | 0.3      | 0.13                | 0.3        |
| (2,881)  | 2:1807:A:LEU:HG   | 2:1801:A:CYS:HB2  | 6                   | 0.3      | 0.14                | 0.29       |
| (2,1572) | 2:1809:A:ILE:HD11 | 2:1805:A:PHE:HD2  | 6                   | 0.3      | 0.26                | 0.2        |
| (2,1572) | 2:1809:A:ILE:HD13 | 2:1805:A:PHE:HD1  | 6                   | 0.3      | 0.26                | 0.2        |
| (2,1572) | 2:1809:A:ILE:HD13 | 2:1805:A:PHE:HD2  | 6                   | 0.3      | 0.26                | 0.2        |
| (2,1572) | 2:1809:A:ILE:HD11 | 2:1805:A:PHE:HD1  | 6                   | 0.3      | 0.26                | 0.2        |
| (2,1572) | 2:1809:A:ILE:HD12 | 2:1805:A:PHE:HD2  | 6                   | 0.3      | 0.26                | 0.2        |
| (2,1069) | 2:1768:A:THR:HG21 | 2:1785:A:LEU:HD23 | 6                   | 0.27     | 0.06                | 0.26       |
| (2,1069) | 2:1768:A:THR:HG23 | 2:1785:A:LEU:HD23 | 6                   | 0.27     | 0.06                | 0.26       |
| (2,1069) | 2:1768:A:THR:HG23 | 2:1785:A:LEU:HD22 | 6                   | 0.27     | 0.06                | 0.26       |
| (2,1069) | 2:1768:A:THR:HG22 | 2:1785:A:LEU:HD22 | 6                   | 0.27     | 0.06                | 0.26       |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG21 | 6                   | 0.26     | 0.08                | 0.27       |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG22 | 6                   | 0.26     | 0.08                | 0.27       |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG23 | 6                   | 0.26     | 0.08                | 0.27       |
| (2,386)  | 1:126:B:LEU:H     | 1:126:B:LEU:HD13  | 6                   | 0.24     | 0.13                | 0.22       |
| (2,386)  | 1:126:B:LEU:H     | 1:126:B:LEU:HD11  | 6                   | 0.24     | 0.13                | 0.22       |
| (2,386)  | 1:126:B:LEU:H     | 1:126:B:LEU:HD12  | 6                   | 0.24     | 0.13                | 0.22       |
| (2,754)  | 2:1774:A:LYS:HG2  | 2:1774:A:LYS:HE3  | 6                   | 0.24     | 0.05                | 0.24       |
| (2,1414) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HB3   | 6                   | 0.21     | 0.04                | 0.21       |
| (2,1414) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HB3   | 6                   | 0.21     | 0.04                | 0.21       |
| (2,1219) | 2:1800:A:LYS:HG3  | 2:1800:A:LYS:HE2  | 6                   | 0.17     | 0.02                | 0.17       |
| (2,569)  | 1:124:B:ILE:HA    | 1:124:B:ILE:HG22  | 6                   | 0.14     | 0.02                | 0.15       |
| (2,569)  | 1:124:B:ILE:HA    | 1:124:B:ILE:HG23  | 6                   | 0.14     | 0.02                | 0.15       |
| (2,472)  | 1:123:B:ILE:H     | 1:123:B:ILE:HD11  | 6                   | 0.14     | 0.07                | 0.11       |
| (2,472)  | 1:123:B:ILE:H     | 1:123:B:ILE:HD12  | 6                   | 0.14     | 0.07                | 0.11       |
| (2,509)  | 1:117:B:ASP:HA    | 1:117:B:ASP:HB3   | 6                   | 0.12     | 0.01                | 0.12       |
| (2,501)  | 1:120:B:ILE:HG12  | 1:120:B:ILE:HA    | 6                   | 0.11     | 0.01                | 0.11       |
| (2,647)  | 1:133:B:GLU:HB3   | 1:131:B:ASN:HD22  | 5                   | 1.42     | 1.53                | 0.31       |
| (2,1101) | 2:1794:A:LYS:HE2  | 2:1791:A:TYR:HA   | 5                   | 1.42     | 0.12                | 1.35       |
| (2,1193) | 2:1775:A:THR:HA   | 2:1774:A:LYS:HG3  | 5                   | 0.82     | 0.62                | 0.57       |
| (2,560)  | 1:134:B:ILE:HD12  | 1:131:B:ASN:HD22  | 5                   | 0.66     | 0.26                | 0.75       |
| (2,560)  | 1:134:B:ILE:HD13  | 1:131:B:ASN:HD22  | 5                   | 0.66     | 0.26                | 0.75       |
| (2,560)  | 1:134:B:ILE:HD11  | 1:131:B:ASN:HD22  | 5                   | 0.66     | 0.26                | 0.75       |
| (2,1432) | 2:1783:A:LYS:HB2  | 2:1783:A:LYS:HE2  | 5                   | 0.63     | 0.25                | 0.75       |
| (2,973)  | 2:1812:A:LYS:HA   | 2:1812:A:LYS:HG2  | 5                   | 0.63     | 0.03                | 0.64       |
| (2,238)  | 2:1779:A:CYS:H    | 2:1773:A:ARG:HD3  | 5                   | 0.54     | 0.62                | 0.21       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1098) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HE2  | 5                   | 0.49     | 0.02                | 0.49       |
| (2,192)  | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG22  | 5                   | 0.47     | 0.32                | 0.41       |
| (2,192)  | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG23  | 5                   | 0.47     | 0.32                | 0.41       |
| (2,192)  | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG21  | 5                   | 0.47     | 0.32                | 0.41       |
| (2,1228) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:HA   | 5                   | 0.46     | 0.04                | 0.48       |
| (2,1099) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HD3  | 5                   | 0.42     | 0.25                | 0.63       |
| (2,750)  | 2:1812:A:LYS:HG2  | 2:1812:A:LYS:H    | 5                   | 0.39     | 0.1                 | 0.36       |
| (2,668)  | 1:120:B:ILE:HD12  | 1:116:B:MET:HA    | 5                   | 0.34     | 0.14                | 0.33       |
| (2,668)  | 1:120:B:ILE:HD13  | 1:116:B:MET:HA    | 5                   | 0.34     | 0.14                | 0.33       |
| (2,387)  | 1:116:B:MET:H     | 1:115:B:GLN:HB2   | 5                   | 0.3      | 0.11                | 0.35       |
| (2,345)  | 1:130:B:TYR:H     | 1:129:B:SER:HB3   | 5                   | 0.28     | 0.01                | 0.28       |
| (2,1677) | 2:1767:A:HIS:HB3  | 2:1781:A:ILE:HG21 | 5                   | 0.27     | 0.06                | 0.27       |
| (2,1677) | 2:1767:A:HIS:HB3  | 2:1781:A:ILE:HG23 | 5                   | 0.27     | 0.06                | 0.27       |
| (2,470)  | 1:125:B:SER:H     | 1:124:B:ILE:HG22  | 5                   | 0.18     | 0.05                | 0.19       |
| (2,470)  | 1:125:B:SER:H     | 1:124:B:ILE:HG23  | 5                   | 0.18     | 0.05                | 0.19       |
| (2,470)  | 1:125:B:SER:H     | 1:124:B:ILE:HG21  | 5                   | 0.18     | 0.05                | 0.19       |
| (2,1637) | 2:1810:A:LYS:HD2  | 2:1810:A:LYS:H    | 5                   | 0.17     | 0.04                | 0.19       |
| (2,969)  | 2:1769:A:LYS:HD3  | 2:1766:A:GLN:HA   | 5                   | 0.16     | 0.03                | 0.15       |
| (2,321)  | 2:1777:A:GLY:H    | 2:1776:A:ASN:HA   | 5                   | 0.15     | 0.03                | 0.14       |
| (2,1006) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HB3  | 5                   | 0.13     | 0.02                | 0.13       |
| (2,826)  | 2:1791:A:TYR:HA   | 2:1794:A:LYS:HB2  | 5                   | 0.13     | 0.04                | 0.12       |
| (2,1179) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:H    | 5                   | 0.13     | 0.02                | 0.13       |
| (2,1179) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:H    | 5                   | 0.13     | 0.02                | 0.13       |
| (2,1179) | 2:1755:A:LEU:HD11 | 2:1755:A:LEU:H    | 5                   | 0.13     | 0.02                | 0.13       |
| (2,598)  | 1:116:B:MET:HA    | 1:116:B:MET:HG3   | 5                   | 0.12     | 0.01                | 0.12       |
| (2,979)  | 2:1757:A:SER:HA   | 2:1760:A:LYS:HB2  | 5                   | 0.12     | 0.01                | 0.12       |
| (2,521)  | 1:137:B:LEU:HD12  | 1:137:B:LEU:HA    | 4                   | 1.12     | 0.43                | 1.16       |
| (2,521)  | 1:137:B:LEU:HD11  | 1:137:B:LEU:HA    | 4                   | 1.12     | 0.43                | 1.16       |
| (2,521)  | 1:137:B:LEU:HD13  | 1:137:B:LEU:HA    | 4                   | 1.12     | 0.43                | 1.16       |
| (2,672)  | 1:129:B:SER:HA    | 1:132:B:GLU:HG2   | 4                   | 0.78     | 0.31                | 0.76       |
| (2,1052) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HE2  | 4                   | 0.62     | 0.14                | 0.62       |
| (2,822)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HG2  | 4                   | 0.54     | 0.02                | 0.55       |
| (2,120)  | 2:1752:A:ASN:H    | 2:1752:A:ASN:HD22 | 4                   | 0.51     | 0.03                | 0.52       |
| (2,559)  | 1:134:B:ILE:HD13  | 1:131:B:ASN:HD21  | 4                   | 0.39     | 0.01                | 0.39       |
| (2,559)  | 1:134:B:ILE:HD11  | 1:131:B:ASN:HD21  | 4                   | 0.39     | 0.01                | 0.39       |
| (2,559)  | 1:134:B:ILE:HD12  | 1:131:B:ASN:HD21  | 4                   | 0.39     | 0.01                | 0.39       |
| (2,1664) | 2:1811:A:GLN:HG3  | 2:1811:A:GLN:H    | 4                   | 0.29     | 0.2                 | 0.2        |
| (2,951)  | 2:1780:A:PRO:HB3  | 1:134:B:ILE:HG21  | 4                   | 0.27     | 0.09                | 0.28       |
| (2,951)  | 2:1780:A:PRO:HB3  | 1:134:B:ILE:HG22  | 4                   | 0.27     | 0.09                | 0.28       |
| (2,998)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HG3  | 4                   | 0.23     | 0.18                | 0.15       |
| (2,427)  | 1:136:B:GLY:H     | 1:135:B:LEU:HG    | 4                   | 0.2      | 0.05                | 0.2        |
| (2,37)   | 2:1766:A:GLN:HE22 | 2:1766:A:GLN:HG2  | 4                   | 0.18     | 0.01                | 0.18       |

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| Key      | Atom-1           | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,786)  | 2:1805:A:PHE:HB2 | 2:1809:A:ILE:HD13 | 4                   | 0.18     | 0.04                | 0.19       |
| (2,786)  | 2:1805:A:PHE:HB2 | 2:1809:A:ILE:HD12 | 4                   | 0.18     | 0.04                | 0.19       |
| (2,786)  | 2:1805:A:PHE:HB2 | 2:1809:A:ILE:HD11 | 4                   | 0.18     | 0.04                | 0.19       |
| (2,1103) | 2:1774:A:LYS:HE3 | 2:1774:A:LYS:HD3  | 4                   | 0.16     | 0.01                | 0.16       |
| (2,1079) | 2:1782:A:CYS:HA  | 2:1781:A:ILE:HG21 | 4                   | 0.16     | 0.01                | 0.16       |
| (2,1079) | 2:1782:A:CYS:HA  | 2:1781:A:ILE:HG22 | 4                   | 0.16     | 0.01                | 0.16       |
| (2,488)  | 1:117:B:ASP:HB3  | 1:120:B:ILE:HG13  | 3                   | 1.2      | 0.1                 | 1.25       |
| (2,1039) | 2:1731:A:ARG:HD2 | 2:1731:A:ARG:HB2  | 3                   | 0.92     | 0.09                | 0.89       |
| (2,554)  | 1:124:B:ILE:HD13 | 1:124:B:ILE:HA    | 3                   | 0.74     | 0.02                | 0.75       |
| (2,554)  | 1:124:B:ILE:HD11 | 1:124:B:ILE:HA    | 3                   | 0.74     | 0.02                | 0.75       |
| (2,671)  | 1:126:B:LEU:HG   | 1:122:B:ASP:HB2   | 3                   | 0.58     | 0.27                | 0.7        |
| (2,915)  | 2:1773:A:ARG:HG2 | 2:1773:A:ARG:HD3  | 3                   | 0.54     | 0.01                | 0.54       |
| (2,275)  | 2:1778:A:GLY:H   | 2:1776:A:ASN:HB2  | 3                   | 0.44     | 0.05                | 0.41       |
| (2,1308) | 2:1811:A:GLN:HB2 | 2:1811:A:GLN:HG3  | 3                   | 0.42     | 0.0                 | 0.42       |
| (2,277)  | 2:1738:A:ALA:H   | 2:1737:A:ARG:HD2  | 3                   | 0.34     | 0.21                | 0.29       |
| (2,987)  | 2:1764:A:VAL:HA  | 2:1781:A:ILE:HG23 | 3                   | 0.31     | 0.08                | 0.31       |
| (2,1089) | 2:1774:A:LYS:HA  | 2:1779:A:CYS:HB2  | 3                   | 0.3      | 0.05                | 0.3        |
| (2,1331) | 2:1811:A:GLN:HB3 | 2:1811:A:GLN:H    | 3                   | 0.26     | 0.08                | 0.32       |
| (2,467)  | 1:124:B:ILE:HG22 | 1:124:B:ILE:HG12  | 3                   | 0.2      | 0.01                | 0.2        |
| (2,467)  | 1:124:B:ILE:HG21 | 1:124:B:ILE:HG12  | 3                   | 0.2      | 0.01                | 0.2        |
| (2,889)  | 2:1741:A:SER:HB3 | 2:1761:A:MET:HG3  | 3                   | 0.2      | 0.09                | 0.15       |
| (2,356)  | 1:121:B:ASP:H    | 1:121:B:ASP:HB3   | 3                   | 0.17     | 0.01                | 0.17       |
| (2,555)  | 1:124:B:ILE:HD11 | 1:124:B:ILE:HB    | 3                   | 0.17     | 0.02                | 0.16       |
| (2,555)  | 1:124:B:ILE:HD12 | 1:124:B:ILE:HB    | 3                   | 0.17     | 0.02                | 0.16       |
| (2,1281) | 2:1736:A:GLN:HG2 | 2:1736:A:GLN:H    | 3                   | 0.15     | 0.04                | 0.13       |
| (2,638)  | 1:115:B:GLN:HG2  | 1:115:B:GLN:HA    | 3                   | 0.15     | 0.03                | 0.14       |
| (2,389)  | 1:116:B:MET:H    | 1:115:B:GLN:HA    | 3                   | 0.14     | 0.01                | 0.14       |
| (1,24)   | 2:1769:A:LYS:H   | 2:1765:A:VAL:O    | 3                   | 0.14     | 0.01                | 0.13       |
| (2,1716) | 2:1785:A:LEU:HB2 | 2:1805:A:PHE:HE1  | 3                   | 0.14     | 0.04                | 0.12       |
| (2,1716) | 2:1785:A:LEU:HB2 | 2:1805:A:PHE:HE2  | 3                   | 0.14     | 0.04                | 0.12       |
| (2,448)  | 1:131:B:ASN:H    | 1:131:B:ASN:HD21  | 3                   | 0.13     | 0.0                 | 0.13       |
| (2,1169) | 2:1741:A:SER:HA  | 2:1744:A:HIS:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (2,868)  | 2:1727:A:PRO:HD3 | 2:1727:A:PRO:HG2  | 3                   | 0.12     | 0.02                | 0.12       |
| (2,1110) | 2:1747:A:GLN:HB2 | 2:1747:A:GLN:H    | 3                   | 0.12     | 0.03                | 0.1        |
| (2,212)  | 2:1740:A:GLN:H   | 2:1743:A:VAL:HG13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,212)  | 2:1740:A:GLN:H   | 2:1743:A:VAL:HG11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,340)  | 1:130:B:TYR:H    | 1:130:B:TYR:HD2   | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,340)  | 1:130:B:TYR:H    | 1:130:B:TYR:HD1   | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,718)  | 2:1787:A:ALA:HB3 | 2:1787:A:ALA:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,718)  | 2:1787:A:ALA:HB2 | 2:1787:A:ALA:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,867)  | 2:1785:A:LEU:HG  | 2:1785:A:LEU:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,1438) | 2:1788:A:LEU:HB3 | 2:1788:A:LEU:H    | 3                   | 0.1      | 0.0                 | 0.1        |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (2,1004) | 2:1738:A:ALA:HB1  | 2:1738:A:ALA:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (2,1004) | 2:1738:A:ALA:HB2  | 2:1738:A:ALA:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (2,1231) | 2:1784:A:GLN:HB3  | 2:1788:A:LEU:HD22 | 2                   | 1.32     | 0.1                 | 1.32       |
| (2,1231) | 2:1784:A:GLN:HB3  | 2:1788:A:LEU:HD21 | 2                   | 1.32     | 0.1                 | 1.32       |
| (2,1223) | 2:1748:A:CYS:HB2  | 2:1762:A:LYS:HE2  | 2                   | 1.28     | 0.01                | 1.28       |
| (2,239)  | 2:1779:A:CYS:H    | 2:1773:A:ARG:HB3  | 2                   | 0.9      | 0.76                | 0.9        |
| (2,802)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:HA   | 2                   | 0.83     | 0.3                 | 0.83       |
| (2,678)  | 1:134:B:ILE:HG22  | 1:131:B:ASN:HD22  | 2                   | 0.5      | 0.26                | 0.5        |
| (2,678)  | 1:134:B:ILE:HG23  | 1:131:B:ASN:HD22  | 2                   | 0.5      | 0.26                | 0.5        |
| (2,1595) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HE22 | 2                   | 0.48     | 0.34                | 0.48       |
| (2,268)  | 2:1773:A:ARG:H    | 2:1773:A:ARG:HD3  | 2                   | 0.47     | 0.01                | 0.47       |
| (2,1639) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:H    | 2                   | 0.47     | 0.03                | 0.47       |
| (2,936)  | 2:1732:A:ARG:HG2  | 2:1732:A:ARG:HA   | 2                   | 0.4      | 0.02                | 0.4        |
| (2,838)  | 2:1745:A:ALA:HA   | 2:1762:A:LYS:HE2  | 2                   | 0.37     | 0.01                | 0.37       |
| (2,429)  | 1:125:B:SER:H     | 1:125:B:SER:HB2   | 2                   | 0.31     | 0.0                 | 0.31       |
| (2,646)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HD2   | 2                   | 0.3      | 0.12                | 0.3        |
| (2,646)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HD1   | 2                   | 0.3      | 0.12                | 0.3        |
| (2,622)  | 1:139:B:ASP:HB3   | 1:140:B:PRO:HD2   | 2                   | 0.27     | 0.03                | 0.27       |
| (2,963)  | 2:1739:A:ILE:HD12 | 2:1792:A:HIS:HB3  | 2                   | 0.27     | 0.13                | 0.27       |
| (2,963)  | 2:1739:A:ILE:HD13 | 2:1792:A:HIS:HB3  | 2                   | 0.27     | 0.13                | 0.27       |
| (2,1640) | 2:1807:A:LEU:HA   | 2:1810:A:LYS:HG3  | 2                   | 0.26     | 0.04                | 0.26       |
| (2,765)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:HE2  | 2                   | 0.23     | 0.11                | 0.23       |
| (2,1093) | 2:1774:A:LYS:HA   | 2:1774:A:LYS:HG3  | 2                   | 0.22     | 0.06                | 0.22       |
| (2,290)  | 2:1773:A:ARG:H    | 2:1773:A:ARG:HG2  | 2                   | 0.2      | 0.09                | 0.2        |
| (2,289)  | 2:1784:A:GLN:HE21 | 2:1784:A:GLN:HB3  | 2                   | 0.2      | 0.05                | 0.2        |
| (2,1158) | 2:1758:A:CYS:HA   | 2:1761:A:MET:HB2  | 2                   | 0.18     | 0.0                 | 0.18       |
| (2,1476) | 2:1805:A:PHE:HB3  | 2:1809:A:ILE:HD11 | 2                   | 0.18     | 0.04                | 0.18       |
| (2,1476) | 2:1805:A:PHE:HB3  | 2:1809:A:ILE:HD13 | 2                   | 0.18     | 0.04                | 0.18       |
| (2,1105) | 2:1774:A:LYS:HE3  | 2:1805:A:PHE:HE2  | 2                   | 0.16     | 0.03                | 0.16       |
| (2,1105) | 2:1774:A:LYS:HE3  | 2:1805:A:PHE:HE1  | 2                   | 0.16     | 0.03                | 0.16       |
| (2,333)  | 1:137:B:LEU:H     | 1:136:B:GLY:H     | 2                   | 0.14     | 0.0                 | 0.14       |
| (2,1471) | 2:1798:A:GLU:HA   | 2:1798:A:GLU:HG2  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,7)    | 2:1785:A:LEU:H    | 2:1784:A:GLN:HB2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (2,526)  | 1:132:B:GLU:HG2   | 1:132:B:GLU:HA    | 2                   | 0.13     | 0.03                | 0.13       |
| (2,1168) | 2:1724:A:THR:HA   | 2:1724:A:THR:HG21 | 2                   | 0.12     | 0.01                | 0.12       |
| (2,1168) | 2:1724:A:THR:HA   | 2:1724:A:THR:HG22 | 2                   | 0.12     | 0.01                | 0.12       |
| (2,1299) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG21 | 2                   | 0.12     | 0.01                | 0.12       |
| (2,1440) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HE2  | 2                   | 0.12     | 0.01                | 0.12       |
| (2,863)  | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1131) | 2:1761:A:MET:HE1  | 2:1742:A:LEU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (2,351)  | 1:133:B:GLU:H     | 1:133:B:GLU:HG3   | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1200) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:H    | 2                   | 0.12     | 0.0                 | 0.12       |

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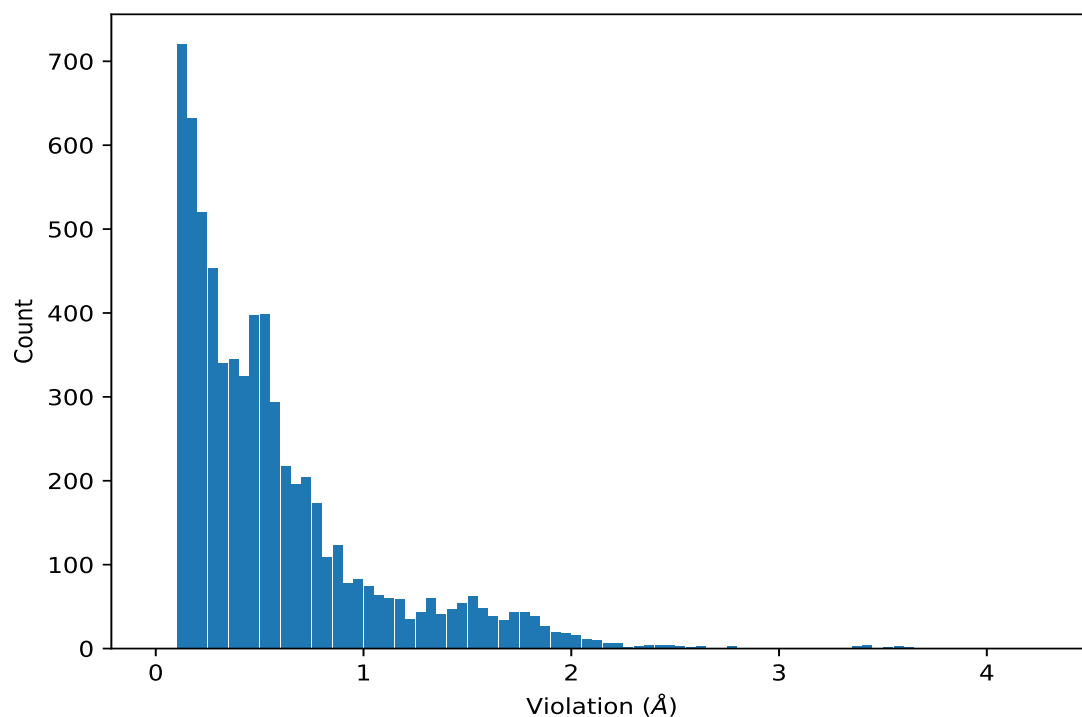
| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,197) | 2:1761:A:MET:H | 2:1759:A:GLN:H | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,511) | 1:119:B:VAL:H  | 1:118:B:ASP:HA | 2                   | 0.11     | 0.01                | 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) |
|---------|------------------|------------------|----------|---------------|
| (2,636) | 1:135:B:LEU:HD21 | 1:132:B:GLU:HB2  | 5        | 4.27          |
| (2,665) | 1:119:B:VAL:HG11 | 1:120:B:ILE:HG13 | 18       | 3.67          |

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| Key      | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|----------|------------------|-------------------|----------|---------------|
| (2,665)  | 1:119:B:VAL:HG13 | 1:120:B:ILE:HG13  | 11       | 3.62          |
| (2,665)  | 1:119:B:VAL:HG13 | 1:120:B:ILE:HG13  | 19       | 3.61          |
| (2,680)  | 1:138:B:MET:HG2  | 1:137:B:LEU:HD11  | 4        | 3.59          |
| (2,665)  | 1:119:B:VAL:HG12 | 1:120:B:ILE:HG13  | 4        | 3.59          |
| (2,637)  | 1:135:B:LEU:HD23 | 1:132:B:GLU:HG2   | 5        | 3.58          |
| (2,665)  | 1:119:B:VAL:HG11 | 1:120:B:ILE:HG13  | 6        | 3.52          |
| (2,665)  | 1:119:B:VAL:HG12 | 1:120:B:ILE:HG13  | 2        | 3.51          |
| (2,665)  | 1:119:B:VAL:HG12 | 1:120:B:ILE:HG13  | 5        | 3.47          |
| (2,665)  | 1:119:B:VAL:HG12 | 1:120:B:ILE:HG13  | 17       | 3.44          |
| (2,665)  | 1:119:B:VAL:HG13 | 1:120:B:ILE:HG13  | 13       | 3.42          |
| (2,665)  | 1:119:B:VAL:HG11 | 1:120:B:ILE:HG13  | 10       | 3.41          |
| (2,665)  | 1:119:B:VAL:HG13 | 1:120:B:ILE:HG13  | 16       | 3.41          |
| (2,665)  | 1:119:B:VAL:HG11 | 1:120:B:ILE:HG13  | 20       | 3.39          |
| (2,665)  | 1:119:B:VAL:HG11 | 1:120:B:ILE:HG13  | 14       | 3.38          |
| (2,680)  | 1:138:B:MET:HG2  | 1:137:B:LEU:HD11  | 10       | 3.36          |
| (2,647)  | 1:133:B:GLU:HB3  | 1:131:B:ASN:HD22  | 9        | 3.33          |
| (2,647)  | 1:133:B:GLU:HB3  | 1:131:B:ASN:HD22  | 2        | 3.25          |
| (2,657)  | 1:135:B:LEU:HD21 | 1:130:B:TYR:HD1   | 5        | 2.84          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 14       | 2.79          |
| (2,971)  | 2:1734:A:SER:HB3 | 2:1733:A:LEU:HD13 | 3        | 2.77          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 8        | 2.75          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 16       | 2.7           |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 2        | 2.68          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD21 | 3        | 2.63          |
| (2,1210) | 2:1784:A:GLN:HG3 | 2:1788:A:LEU:HD23 | 19       | 2.6           |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD22 | 10       | 2.6           |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 1        | 2.58          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD21 | 6        | 2.56          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 9        | 2.53          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD22 | 18       | 2.53          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 15       | 2.52          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD21 | 20       | 2.49          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD22 | 17       | 2.48          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD21 | 19       | 2.48          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD22 | 13       | 2.47          |
| (2,1000) | 2:1738:A:ALA:HB1 | 2:1788:A:LEU:HD13 | 7        | 2.44          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD22 | 4        | 2.43          |
| (2,1210) | 2:1784:A:GLN:HG3 | 2:1788:A:LEU:HD23 | 6        | 2.4           |
| (2,561)  | 1:119:B:VAL:HG21 | 1:118:B:ASP:HB3   | 13       | 2.4           |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD22 | 5        | 2.39          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 12       | 2.39          |
| (2,1015) | 2:1735:A:ILE:HB  | 2:1788:A:LEU:HD23 | 7        | 2.36          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,561)  | 1:119:B:VAL:HG22  | 1:118:B:ASP:HB3   | 9        | 2.36          |
| (2,1015) | 2:1735:A:ILE:HB   | 2:1788:A:LEU:HD21 | 11       | 2.33          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 10       | 2.32          |
| (2,561)  | 1:119:B:VAL:HG23  | 1:118:B:ASP:HB3   | 15       | 2.32          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD21 | 4        | 2.29          |
| (2,561)  | 1:119:B:VAL:HG22  | 1:118:B:ASP:HB3   | 17       | 2.28          |
| (2,561)  | 1:119:B:VAL:HG22  | 1:118:B:ASP:HB3   | 12       | 2.24          |
| (2,1404) | 2:1788:A:LEU:HD12 | 2:1739:A:ILE:H    | 7        | 2.23          |
| (2,561)  | 1:119:B:VAL:HG22  | 1:118:B:ASP:HB3   | 11       | 2.22          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 14       | 2.2           |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD21 | 13       | 2.2           |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 2        | 2.2           |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD22 | 1        | 2.17          |
| (2,561)  | 1:119:B:VAL:HG23  | 1:118:B:ASP:HB3   | 19       | 2.17          |
| (2,665)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:HG13  | 1        | 2.16          |
| (2,561)  | 1:119:B:VAL:HG23  | 1:118:B:ASP:HB3   | 6        | 2.16          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD22 | 14       | 2.15          |
| (2,850)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB3  | 19       | 2.15          |
| (2,1404) | 2:1788:A:LEU:HD12 | 2:1739:A:ILE:H    | 19       | 2.14          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 1        | 2.13          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 5        | 2.13          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 7        | 2.13          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 13       | 2.13          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD22 | 8        | 2.13          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD22 | 16       | 2.13          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 10       | 2.11          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 11       | 2.11          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 2        | 2.1           |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 3        | 2.09          |
| (2,513)  | 1:126:B:LEU:HD12  | 1:123:B:ILE:HA    | 9        | 2.09          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD21 | 18       | 2.08          |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD12 | 19       | 2.08          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD22 | 2        | 2.07          |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 20       | 2.06          |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD13 | 20       | 2.06          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 2        | 2.05          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 3        | 2.05          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD21 | 10       | 2.05          |
| (2,561)  | 1:119:B:VAL:HG22  | 1:118:B:ASP:HB3   | 4        | 2.05          |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD1  | 14       | 2.04          |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 4        | 2.04          |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD12 | 11       | 2.04          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD2  | 17       | 2.03          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 8        | 2.03          |
| (2,561)  | 1:119:B:VAL:HG23  | 1:118:B:ASP:HB3   | 3        | 2.03          |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD1  | 8        | 2.02          |
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD1  | 13       | 2.02          |
| (2,1634) | 2:1788:A:LEU:HD22 | 2:1791:A:TYR:HD2  | 20       | 2.02          |
| (2,1404) | 2:1788:A:LEU:HD12 | 2:1739:A:ILE:H    | 2        | 2.02          |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD13 | 2        | 2.02          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 14       | 2.02          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 17       | 2.01          |
| (2,1634) | 2:1788:A:LEU:HD22 | 2:1791:A:TYR:HD2  | 6        | 2.0           |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 15       | 2.0           |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD23 | 3        | 2.0           |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 8        | 1.99          |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 14       | 1.99          |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 13       | 1.99          |
| (2,666)  | 1:120:B:ILE:HD11  | 1:117:B:ASP:HB3   | 9        | 1.99          |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 2        | 1.97          |
| (2,1634) | 2:1788:A:LEU:HD22 | 2:1791:A:TYR:HD1  | 3        | 1.97          |
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD1  | 10       | 1.97          |
| (2,1634) | 2:1788:A:LEU:HD22 | 2:1791:A:TYR:HD1  | 19       | 1.97          |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 7        | 1.97          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD23 | 9        | 1.97          |
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD1  | 18       | 1.96          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 10       | 1.96          |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD11 | 13       | 1.96          |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD13  | 8        | 1.96          |
| (2,665)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:HG13  | 7        | 1.96          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 1        | 1.96          |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 15       | 1.95          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD23 | 11       | 1.95          |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD11 | 17       | 1.95          |
| (2,1500) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HD3  | 1        | 1.94          |
| (2,1404) | 2:1788:A:LEU:HD13 | 2:1739:A:ILE:H    | 20       | 1.94          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 10       | 1.94          |
| (2,513)  | 1:126:B:LEU:HD12  | 1:123:B:ILE:HA    | 3        | 1.94          |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 7        | 1.93          |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 16       | 1.93          |
| (2,1500) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HD3  | 19       | 1.93          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 15       | 1.92          |
| (2,1634) | 2:1788:A:LEU:HD22 | 2:1791:A:TYR:HD2  | 11       | 1.92          |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 18       | 1.92          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD23 | 15       | 1.92          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD21 | 20       | 1.92          |
| (2,665)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:HG13  | 12       | 1.92          |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 9        | 1.91          |
| (2,1404) | 2:1788:A:LEU:HD12 | 2:1739:A:ILE:H    | 11       | 1.91          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD21 | 6        | 1.91          |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 1        | 1.9           |
| (2,1500) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HD3  | 5        | 1.9           |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD12  | 9        | 1.9           |
| (2,665)  | 1:119:B:VAL:HG11  | 1:120:B:ILE:HG13  | 8        | 1.9           |
| (2,1634) | 2:1788:A:LEU:HD21 | 2:1791:A:TYR:HD2  | 12       | 1.89          |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 16       | 1.89          |
| (2,1404) | 2:1788:A:LEU:HD12 | 2:1739:A:ILE:H    | 18       | 1.89          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 14       | 1.89          |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD12 | 18       | 1.89          |
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD2  | 4        | 1.88          |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 2        | 1.88          |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD13 | 4        | 1.88          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 1        | 1.88          |
| (2,665)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:HG13  | 9        | 1.88          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 13       | 1.87          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 14       | 1.87          |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 7        | 1.86          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 12       | 1.86          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD21 | 5        | 1.86          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 9        | 1.86          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 16       | 1.86          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD23 | 19       | 1.86          |
| (2,851)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB2  | 13       | 1.86          |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 6        | 1.85          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD21 | 2        | 1.85          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 1        | 1.85          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 10       | 1.85          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 17       | 1.85          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 18       | 1.85          |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD11 | 6        | 1.85          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD21 | 4        | 1.85          |
| (2,1634) | 2:1788:A:LEU:HD23 | 2:1791:A:TYR:HD1  | 5        | 1.84          |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 17       | 1.84          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 13       | 1.84          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 18       | 1.84          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 4        | 1.84          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD21 | 8        | 1.84          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 15       | 1.84          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 19       | 1.84          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 20       | 1.84          |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD11 | 10       | 1.84          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 8        | 1.84          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 4        | 1.84          |
| (2,513)  | 1:126:B:LEU:HD11  | 1:123:B:ILE:HA    | 1        | 1.84          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD21 | 2        | 1.83          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD23 | 3        | 1.83          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD21 | 5        | 1.83          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 7        | 1.83          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 11       | 1.83          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD22 | 16       | 1.83          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD23 | 6        | 1.83          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 12       | 1.83          |
| (2,1404) | 2:1788:A:LEU:HD13 | 2:1739:A:ILE:H    | 4        | 1.82          |
| (2,1304) | 2:1751:A:ALA:HB1  | 2:1752:A:ASN:HB2  | 10       | 1.82          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD21 | 6        | 1.82          |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD11 | 14       | 1.82          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 2        | 1.82          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD23 | 3        | 1.82          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD21 | 13       | 1.82          |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 2        | 1.81          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 19       | 1.81          |
| (2,1024) | 2:1742:A:LEU:HA   | 2:1742:A:LEU:HD21 | 9        | 1.81          |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 3        | 1.8           |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD13 | 8        | 1.8           |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 9        | 1.8           |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 8        | 1.8           |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 20       | 1.8           |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 7        | 1.8           |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD21 | 10       | 1.8           |
| (2,513)  | 1:126:B:LEU:HD13  | 1:123:B:ILE:HA    | 16       | 1.8           |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 16       | 1.79          |
| (2,1404) | 2:1788:A:LEU:HD12 | 2:1739:A:ILE:H    | 3        | 1.79          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 7        | 1.79          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 18       | 1.79          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 8        | 1.78          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 9        | 1.78          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 3        | 1.78          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD11 | 4        | 1.78          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 10       | 1.78          |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 13       | 1.78          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 10       | 1.78          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD21 | 18       | 1.78          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 9        | 1.78          |
| (2,850)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB3  | 3        | 1.78          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 1        | 1.77          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 2        | 1.77          |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 6        | 1.77          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD11 | 13       | 1.77          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 13       | 1.77          |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD13 | 15       | 1.77          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD22 | 17       | 1.77          |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 20       | 1.77          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 5        | 1.76          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 12       | 1.76          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 16       | 1.76          |
| (2,1359) | 2:1742:A:LEU:HD13 | 2:1739:A:ILE:HA   | 11       | 1.76          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD23 | 11       | 1.76          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 15       | 1.76          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD21 | 17       | 1.76          |
| (2,238)  | 2:1779:A:CYS:H    | 2:1773:A:ARG:HD3  | 5        | 1.76          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 4        | 1.75          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 10       | 1.75          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 12       | 1.75          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 14       | 1.75          |
| (2,1500) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HD3  | 12       | 1.75          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD11 | 1        | 1.75          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD13 | 11       | 1.75          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 17       | 1.75          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD13 | 18       | 1.75          |
| (2,1404) | 2:1788:A:LEU:HD13 | 2:1739:A:ILE:H    | 14       | 1.75          |
| (2,1404) | 2:1788:A:LEU:HD13 | 2:1739:A:ILE:H    | 15       | 1.75          |
| (2,1359) | 2:1742:A:LEU:HD13 | 2:1739:A:ILE:HA   | 15       | 1.75          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 12       | 1.75          |
| (2,665)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:HG13  | 15       | 1.75          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 6        | 1.74          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 18       | 1.74          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 19       | 1.74          |
| (2,1500) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HD3  | 9        | 1.74          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 2        | 1.74          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 19       | 1.74          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD11 | 20       | 1.74          |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 9        | 1.74          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 11       | 1.74          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD22 | 14       | 1.74          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 8        | 1.74          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 5        | 1.73          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 13       | 1.73          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD13 | 6        | 1.73          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 17       | 1.73          |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 9        | 1.73          |
| (2,1359) | 2:1742:A:LEU:HD13 | 2:1739:A:ILE:HA   | 1        | 1.73          |
| (2,1359) | 2:1742:A:LEU:HD13 | 2:1739:A:ILE:HA   | 13       | 1.73          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 16       | 1.73          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 7        | 1.72          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 17       | 1.72          |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 5        | 1.72          |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 8        | 1.72          |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 17       | 1.72          |
| (2,975)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HD23 | 20       | 1.72          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 10       | 1.72          |
| (2,1729) | 2:1791:A:TYR:HD1  | 2:1788:A:LEU:HB2  | 3        | 1.71          |
| (2,1654) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HG3  | 5        | 1.71          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 15       | 1.71          |
| (2,1402) | 2:1788:A:LEU:HD13 | 2:1785:A:LEU:HA   | 11       | 1.71          |
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD22 | 17       | 1.71          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD21 | 5        | 1.71          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 17       | 1.71          |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD12 | 3        | 1.71          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 3        | 1.71          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 15       | 1.7           |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 20       | 1.7           |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD11 | 10       | 1.7           |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 19       | 1.7           |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 12       | 1.7           |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD11 | 5        | 1.7           |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 3        | 1.7           |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 16       | 1.7           |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 18       | 1.7           |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 13       | 1.69          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 10       | 1.69          |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 6        | 1.69          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 15       | 1.69          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD22 | 13       | 1.69          |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE2   | 8        | 1.69          |
| (2,1729) | 2:1791:A:TYR:HD2  | 2:1788:A:LEU:HB2  | 11       | 1.68          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD12 | 14       | 1.68          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD21 | 9        | 1.68          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 2        | 1.67          |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 8        | 1.67          |
| (2,1500) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HD3  | 20       | 1.67          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 3        | 1.67          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 18       | 1.67          |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 20       | 1.67          |
| (2,922)  | 2:1765:A:VAL:HG23 | 2:1804:A:PRO:HG2  | 11       | 1.67          |
| (2,487)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 17       | 1.67          |
| (2,1693) | 2:1755:A:LEU:HD12 | 2:1754:A:SER:HB2  | 15       | 1.66          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 11       | 1.66          |
| (2,1500) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HD3  | 10       | 1.66          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 2        | 1.66          |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 14       | 1.66          |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 15       | 1.66          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 1        | 1.66          |
| (2,239)  | 2:1779:A:CYS:H    | 2:1773:A:ARG:HB3  | 3        | 1.66          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 7        | 1.65          |
| (2,1443) | 2:1791:A:TYR:HB2  | 2:1739:A:ILE:HD13 | 7        | 1.65          |
| (2,1404) | 2:1788:A:LEU:HD13 | 2:1739:A:ILE:H    | 16       | 1.65          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 9        | 1.65          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 18       | 1.65          |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD11 | 12       | 1.65          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 5        | 1.65          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 6        | 1.65          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 19       | 1.65          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 13       | 1.64          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 5        | 1.64          |
| (2,1654) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HG3  | 15       | 1.64          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 15       | 1.64          |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 12       | 1.64          |
| (2,1402) | 2:1788:A:LEU:HD13 | 2:1785:A:LEU:HA   | 3        | 1.64          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 4        | 1.64          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 8        | 1.64          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 16       | 1.64          |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 11       | 1.64          |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 4        | 1.63          |
| (2,1383) | 2:1785:A:LEU:HD11 | 2:1785:A:LEU:HA   | 10       | 1.63          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1359) | 2:1742:A:LEU:HD11 | 2:1739:A:ILE:HA   | 14       | 1.63          |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 5        | 1.63          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD21 | 8        | 1.63          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 20       | 1.63          |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE2   | 1        | 1.63          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 17       | 1.62          |
| (2,1383) | 2:1785:A:LEU:HD11 | 2:1785:A:LEU:HA   | 17       | 1.62          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 7        | 1.62          |
| (2,1359) | 2:1742:A:LEU:HD13 | 2:1739:A:ILE:HA   | 12       | 1.62          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 15       | 1.62          |
| (2,1193) | 2:1775:A:THR:HA   | 2:1774:A:LYS:HG3  | 13       | 1.62          |
| (2,1654) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HG3  | 2        | 1.61          |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 1        | 1.61          |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 16       | 1.61          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 5        | 1.61          |
| (2,1101) | 2:1794:A:LYS:HE2  | 2:1791:A:TYR:HA   | 7        | 1.61          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 13       | 1.61          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 8        | 1.61          |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 10       | 1.61          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 7        | 1.6           |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 6        | 1.6           |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 18       | 1.6           |
| (2,1383) | 2:1785:A:LEU:HD12 | 2:1785:A:LEU:HA   | 8        | 1.6           |
| (2,1359) | 2:1742:A:LEU:HD11 | 2:1739:A:ILE:HA   | 17       | 1.6           |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 18       | 1.6           |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 4        | 1.6           |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 12       | 1.6           |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 14       | 1.59          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 5        | 1.59          |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 15       | 1.59          |
| (2,1383) | 2:1785:A:LEU:HD12 | 2:1785:A:LEU:HA   | 4        | 1.59          |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 9        | 1.59          |
| (2,1359) | 2:1742:A:LEU:HD13 | 2:1739:A:ILE:HA   | 19       | 1.59          |
| (2,828)  | 2:1734:A:SER:HA   | 2:1733:A:LEU:HD13 | 3        | 1.59          |
| (2,1693) | 2:1755:A:LEU:HD11 | 2:1754:A:SER:HB2  | 16       | 1.58          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 18       | 1.58          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 19       | 1.58          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 4        | 1.58          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 19       | 1.58          |
| (2,1383) | 2:1785:A:LEU:HD12 | 2:1785:A:LEU:HA   | 13       | 1.58          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 16       | 1.58          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 14       | 1.58          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 20       | 1.58          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 4        | 1.58          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 20       | 1.58          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 14       | 1.58          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 19       | 1.58          |
| (2,522)  | 1:135:B:LEU:HD11  | 1:135:B:LEU:HA    | 5        | 1.58          |
| (2,487)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 9        | 1.58          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 5        | 1.57          |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 7        | 1.57          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 9        | 1.57          |
| (2,922)  | 2:1765:A:VAL:HG23 | 2:1804:A:PRO:HG2  | 9        | 1.57          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 16       | 1.57          |
| (2,850)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB3  | 14       | 1.57          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 9        | 1.57          |
| (2,752)  | 2:1785:A:LEU:HD22 | 2:1786:A:ILE:H    | 20       | 1.57          |
| (2,1693) | 2:1755:A:LEU:HD11 | 2:1754:A:SER:HB2  | 20       | 1.56          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 12       | 1.56          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 6        | 1.56          |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 4        | 1.56          |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 11       | 1.56          |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD13 | 16       | 1.56          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 7        | 1.56          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD21 | 14       | 1.56          |
| (2,752)  | 2:1785:A:LEU:HD21 | 2:1786:A:ILE:H    | 19       | 1.56          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 19       | 1.55          |
| (2,1383) | 2:1785:A:LEU:HD11 | 2:1785:A:LEU:HA   | 6        | 1.55          |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 14       | 1.55          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 13       | 1.55          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 6        | 1.55          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD22 | 11       | 1.55          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 20       | 1.55          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 15       | 1.55          |
| (2,521)  | 1:137:B:LEU:HD11  | 1:137:B:LEU:HA    | 10       | 1.55          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 13       | 1.54          |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 17       | 1.54          |
| (2,1404) | 2:1788:A:LEU:HD11 | 2:1739:A:ILE:H    | 8        | 1.54          |
| (2,1402) | 2:1788:A:LEU:HD13 | 2:1785:A:LEU:HA   | 18       | 1.54          |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 20       | 1.54          |
| (2,1359) | 2:1742:A:LEU:HD11 | 2:1739:A:ILE:HA   | 8        | 1.54          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 7        | 1.54          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 18       | 1.54          |
| (2,922)  | 2:1765:A:VAL:HG22 | 2:1804:A:PRO:HG2  | 2        | 1.54          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,636)  | 1:135:B:LEU:HD22  | 1:132:B:GLU:HB2   | 4        | 1.54          |
| (2,620)  | 1:135:B:LEU:HD21  | 1:130:B:TYR:HE1   | 5        | 1.54          |
| (2,521)  | 1:137:B:LEU:HD11  | 1:137:B:LEU:HA    | 4        | 1.54          |
| (2,487)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 13       | 1.54          |
| (2,487)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 20       | 1.54          |
| (2,1654) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HG3  | 8        | 1.53          |
| (2,1654) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HG3  | 13       | 1.53          |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 19       | 1.53          |
| (2,1304) | 2:1751:A:ALA:HB2  | 2:1752:A:ASN:HB2  | 12       | 1.53          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 13       | 1.53          |
| (2,752)  | 2:1785:A:LEU:HD22 | 2:1786:A:ILE:H    | 13       | 1.53          |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 14       | 1.53          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 20       | 1.53          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 18       | 1.52          |
| (2,1654) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HG3  | 1        | 1.52          |
| (2,1654) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HG3  | 7        | 1.52          |
| (2,1654) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HG3  | 10       | 1.52          |
| (2,1654) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HG3  | 16       | 1.52          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 18       | 1.52          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 8        | 1.52          |
| (2,1500) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HD3  | 11       | 1.52          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 8        | 1.52          |
| (2,1304) | 2:1751:A:ALA:HB1  | 2:1752:A:ASN:HB2  | 3        | 1.52          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 8        | 1.52          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 9        | 1.52          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 12       | 1.52          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD21 | 19       | 1.52          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 7        | 1.52          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 10       | 1.52          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 18       | 1.52          |
| (2,851)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB2  | 20       | 1.52          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 8        | 1.52          |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 17       | 1.52          |
| (2,1693) | 2:1755:A:LEU:HD12 | 2:1754:A:SER:HB2  | 11       | 1.51          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 12       | 1.51          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 1        | 1.51          |
| (2,1193) | 2:1775:A:THR:HA   | 2:1774:A:LYS:HG3  | 17       | 1.51          |
| (2,1066) | 2:1761:A:MET:HG2  | 2:1742:A:LEU:HD23 | 3        | 1.51          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 17       | 1.51          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 4        | 1.51          |
| (2,636)  | 1:135:B:LEU:HD22  | 1:132:B:GLU:HB2   | 9        | 1.51          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 13       | 1.51          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 7        | 1.5           |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 19       | 1.5           |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 2        | 1.5           |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 4        | 1.5           |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 10       | 1.5           |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 2        | 1.5           |
| (2,922)  | 2:1765:A:VAL:HG22 | 2:1804:A:PRO:HG2  | 13       | 1.5           |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 15       | 1.5           |
| (2,752)  | 2:1785:A:LEU:HD21 | 2:1786:A:ILE:H    | 14       | 1.5           |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE1   | 7        | 1.5           |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 3        | 1.5           |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 12       | 1.5           |
| (2,1402) | 2:1788:A:LEU:HD11 | 2:1785:A:LEU:HA   | 16       | 1.49          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 1        | 1.49          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 9        | 1.49          |
| (2,1101) | 2:1794:A:LYS:HE2  | 2:1791:A:TYR:HA   | 17       | 1.49          |
| (2,1000) | 2:1738:A:ALA:HB2  | 2:1788:A:LEU:HD11 | 8        | 1.49          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 10       | 1.49          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 14       | 1.49          |
| (2,850)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB3  | 2        | 1.49          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 9        | 1.49          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 6        | 1.48          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 3        | 1.48          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 18       | 1.48          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 19       | 1.48          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 17       | 1.48          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD23 | 10       | 1.48          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 10       | 1.48          |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD11  | 12       | 1.48          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 4        | 1.47          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 10       | 1.47          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 16       | 1.47          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 15       | 1.47          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 16       | 1.47          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD21 | 6        | 1.47          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 1        | 1.47          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 17       | 1.47          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 1        | 1.47          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 10       | 1.46          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 16       | 1.46          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 17       | 1.46          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 2        | 1.46          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 5        | 1.46          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 13       | 1.46          |
| (2,1135) | 2:1765:A:VAL:HG12 | 2:1804:A:PRO:HG2  | 9        | 1.46          |
| (2,922)  | 2:1765:A:VAL:HG22 | 2:1804:A:PRO:HG2  | 4        | 1.46          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 4        | 1.45          |
| (2,1654) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HG3  | 9        | 1.45          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 7        | 1.45          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 5        | 1.45          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 7        | 1.45          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 16       | 1.45          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 20       | 1.45          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 18       | 1.45          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD23 | 9        | 1.45          |
| (2,1000) | 2:1738:A:ALA:HB3  | 2:1788:A:LEU:HD11 | 1        | 1.45          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD22 | 20       | 1.45          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 18       | 1.45          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 14       | 1.45          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 9        | 1.45          |
| (2,752)  | 2:1785:A:LEU:HD21 | 2:1786:A:ILE:H    | 6        | 1.45          |
| (2,752)  | 2:1785:A:LEU:HD22 | 2:1786:A:ILE:H    | 17       | 1.45          |
| (2,636)  | 1:135:B:LEU:HD21  | 1:132:B:GLU:HB2   | 6        | 1.45          |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 12       | 1.45          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 5        | 1.45          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 7        | 1.45          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD22 | 3        | 1.44          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD22 | 19       | 1.44          |
| (2,1654) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HG3  | 6        | 1.44          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 14       | 1.44          |
| (2,1404) | 2:1788:A:LEU:HD13 | 2:1739:A:ILE:H    | 9        | 1.44          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 3        | 1.44          |
| (2,1276) | 2:1780:A:PRO:HG3  | 2:1781:A:ILE:HG12 | 11       | 1.44          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 2        | 1.44          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 4        | 1.44          |
| (2,850)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB3  | 9        | 1.44          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 19       | 1.44          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 10       | 1.44          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD22 | 2        | 1.43          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD22 | 15       | 1.43          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD21 | 18       | 1.43          |
| (2,1231) | 2:1784:A:GLN:HB3  | 2:1788:A:LEU:HD21 | 5        | 1.43          |
| (2,1135) | 2:1765:A:VAL:HG11 | 2:1804:A:PRO:HG2  | 20       | 1.43          |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 1        | 1.43          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 20       | 1.43          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 18       | 1.43          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 20       | 1.43          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD23 | 5        | 1.42          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD23 | 13       | 1.42          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD21 | 20       | 1.42          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 3        | 1.42          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 3        | 1.42          |
| (2,1135) | 2:1765:A:VAL:HG11 | 2:1804:A:PRO:HG2  | 16       | 1.42          |
| (2,1133) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:HG2  | 14       | 1.42          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD23 | 4        | 1.42          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 14       | 1.42          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD23 | 16       | 1.41          |
| (2,1359) | 2:1742:A:LEU:HD12 | 2:1739:A:ILE:HA   | 5        | 1.41          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 4        | 1.41          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 2        | 1.41          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 7        | 1.41          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 16       | 1.41          |
| (2,752)  | 2:1785:A:LEU:HD21 | 2:1786:A:ILE:H    | 7        | 1.41          |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD21 | 7        | 1.4           |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD23 | 9        | 1.4           |
| (2,1701) | 2:1756:A:PRO:HG3  | 2:1755:A:LEU:HD23 | 11       | 1.4           |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 9        | 1.4           |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD23 | 8        | 1.4           |
| (2,958)  | 2:1760:A:LYS:HA   | 2:1763:A:ARG:HD2  | 17       | 1.4           |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 9        | 1.4           |
| (2,850)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB3  | 16       | 1.4           |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 13       | 1.4           |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 15       | 1.4           |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 12       | 1.39          |
| (2,1402) | 2:1788:A:LEU:HD12 | 2:1785:A:LEU:HA   | 1        | 1.39          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 16       | 1.39          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD21 | 4        | 1.39          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD21 | 7        | 1.39          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 10       | 1.39          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 13       | 1.39          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 7        | 1.39          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 4        | 1.39          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 7        | 1.38          |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD1   | 8        | 1.38          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 5        | 1.38          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 13       | 1.38          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,513)  | 1:126:B:LEU:HD11  | 1:123:B:ILE:HA    | 14       | 1.38          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 16       | 1.38          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 19       | 1.38          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 5        | 1.37          |
| (2,1135) | 2:1765:A:VAL:HG11 | 2:1804:A:PRO:HG2  | 10       | 1.37          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 16       | 1.37          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 15       | 1.37          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 6        | 1.36          |
| (2,1402) | 2:1788:A:LEU:HD13 | 2:1785:A:LEU:HA   | 19       | 1.36          |
| (2,1359) | 2:1742:A:LEU:HD11 | 2:1739:A:ILE:HA   | 4        | 1.36          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 9        | 1.36          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD21 | 20       | 1.36          |
| (2,1133) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:HG2  | 4        | 1.36          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 6        | 1.36          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 19       | 1.36          |
| (2,850)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB3  | 7        | 1.36          |
| (2,529)  | 1:132:B:GLU:HG2   | 1:130:B:TYR:HE2   | 15       | 1.36          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 6        | 1.36          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 18       | 1.36          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 15       | 1.35          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 2        | 1.35          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 1        | 1.35          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 7        | 1.35          |
| (2,1101) | 2:1794:A:LYS:HE2  | 2:1791:A:TYR:HA   | 6        | 1.35          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD21 | 14       | 1.35          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 14       | 1.35          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 8        | 1.35          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 8        | 1.35          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 8        | 1.34          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 13       | 1.34          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 11       | 1.34          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD23 | 3        | 1.34          |
| (2,1135) | 2:1765:A:VAL:HG11 | 2:1804:A:PRO:HG2  | 13       | 1.34          |
| (2,1101) | 2:1794:A:LYS:HE2  | 2:1791:A:TYR:HA   | 15       | 1.34          |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 19       | 1.33          |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 5        | 1.33          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 9        | 1.33          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 17       | 1.33          |
| (2,1359) | 2:1742:A:LEU:HD11 | 2:1739:A:ILE:HA   | 6        | 1.33          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 15       | 1.33          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD22 | 13       | 1.33          |
| (2,1000) | 2:1738:A:ALA:HB1  | 2:1788:A:LEU:HD13 | 9        | 1.33          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 5        | 1.33          |
| (2,676)  | 1:132:B:GLU:HG2   | 1:135:B:LEU:HB2   | 15       | 1.33          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 3        | 1.33          |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 2        | 1.33          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 2        | 1.32          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 7        | 1.32          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 4        | 1.32          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 9        | 1.32          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 20       | 1.32          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 8        | 1.32          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD22 | 1        | 1.32          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD22 | 9        | 1.32          |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 19       | 1.32          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 3        | 1.32          |
| (2,851)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB2  | 4        | 1.32          |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD11  | 19       | 1.32          |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 5        | 1.31          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 6        | 1.31          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 9        | 1.31          |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 10       | 1.31          |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 14       | 1.31          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 15       | 1.31          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 17       | 1.31          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 9        | 1.31          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 6        | 1.31          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD23 | 7        | 1.31          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD22 | 13       | 1.31          |
| (2,1133) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:HG2  | 9        | 1.31          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD22 | 17       | 1.31          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 11       | 1.31          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 1        | 1.3           |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 13       | 1.3           |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 16       | 1.3           |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 18       | 1.3           |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 2        | 1.3           |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 10       | 1.3           |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 18       | 1.3           |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 11       | 1.3           |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD22 | 10       | 1.3           |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD23 | 14       | 1.3           |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD1   | 4        | 1.3           |
| (2,1101) | 2:1794:A:LYS:HE2  | 2:1791:A:TYR:HA   | 5        | 1.3           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD22 | 20       | 1.3           |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 7        | 1.3           |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 1        | 1.3           |
| (2,189)  | 2:1736:A:GLN:H    | 2:1737:A:ARG:HG3  | 11       | 1.3           |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 4        | 1.29          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 20       | 1.29          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 13       | 1.29          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 7        | 1.29          |
| (2,1223) | 2:1748:A:CYS:HB2  | 2:1762:A:LYS:HE2  | 11       | 1.29          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD22 | 2        | 1.29          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD21 | 16       | 1.29          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD23 | 19       | 1.29          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD21 | 6        | 1.29          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD21 | 7        | 1.29          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 5        | 1.29          |
| (2,488)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HG13  | 17       | 1.29          |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 3        | 1.28          |
| (2,1720) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG12 | 8        | 1.28          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 11       | 1.28          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 14       | 1.28          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 14       | 1.28          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 19       | 1.28          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 2        | 1.28          |
| (2,1223) | 2:1748:A:CYS:HB2  | 2:1762:A:LYS:HE2  | 20       | 1.28          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 17       | 1.28          |
| (2,850)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB3  | 1        | 1.28          |
| (2,676)  | 1:132:B:GLU:HG2   | 1:135:B:LEU:HB2   | 3        | 1.28          |
| (2,1720) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG12 | 12       | 1.27          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 18       | 1.27          |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 20       | 1.27          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 8        | 1.27          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 18       | 1.27          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 2        | 1.26          |
| (2,1566) | 2:1794:A:LYS:HB2  | 2:1795:A:HIS:HB2  | 13       | 1.26          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 4        | 1.26          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 3        | 1.26          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 11       | 1.26          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 15       | 1.26          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 18       | 1.26          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 9        | 1.26          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 4        | 1.26          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 2        | 1.26          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD21 | 19       | 1.26          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 19       | 1.25          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 15       | 1.25          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 12       | 1.25          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2  | 4        | 1.25          |
| (2,488)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HG13  | 20       | 1.25          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 5        | 1.24          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 5        | 1.24          |
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 12       | 1.24          |
| (2,672)  | 1:129:B:SER:HA    | 1:132:B:GLU:HG2   | 7        | 1.24          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG13 | 14       | 1.24          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 10       | 1.23          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 18       | 1.23          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 19       | 1.23          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 9        | 1.23          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 9        | 1.23          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 17       | 1.23          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 15       | 1.23          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 1        | 1.23          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 19       | 1.23          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 6        | 1.22          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 4        | 1.22          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 8        | 1.22          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 16       | 1.22          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 19       | 1.22          |
| (2,1231) | 2:1784:A:GLN:HB3  | 2:1788:A:LEU:HD22 | 12       | 1.22          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 4        | 1.21          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 7        | 1.21          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 11       | 1.21          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 10       | 1.21          |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 19       | 1.21          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG12 | 20       | 1.21          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 8        | 1.2           |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 9        | 1.2           |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 1        | 1.2           |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 6        | 1.2           |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 6        | 1.2           |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 3        | 1.2           |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD13  | 1        | 1.2           |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG12 | 15       | 1.2           |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 18       | 1.2           |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 16       | 1.19          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 19       | 1.19          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 14       | 1.19          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 4        | 1.19          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 2        | 1.19          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 10       | 1.19          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 12       | 1.19          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 6        | 1.19          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD11  | 3        | 1.19          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 9        | 1.19          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 12       | 1.19          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 13       | 1.19          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 18       | 1.18          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 1        | 1.18          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 20       | 1.18          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 17       | 1.18          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 8        | 1.18          |
| (2,524)  | 1:137:B:LEU:HD13  | 1:137:B:LEU:HB2   | 15       | 1.18          |
| (2,524)  | 1:137:B:LEU:HD11  | 1:137:B:LEU:HB2   | 20       | 1.18          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 4        | 1.18          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG13 | 11       | 1.18          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 5        | 1.17          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 7        | 1.17          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 17       | 1.17          |
| (2,1704) | 2:1801:A:CYS:HB2  | 2:1807:A:LEU:H    | 20       | 1.17          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 19       | 1.17          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 5        | 1.17          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 12       | 1.17          |
| (2,1135) | 2:1765:A:VAL:HG12 | 2:1804:A:PRO:HG2  | 4        | 1.17          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 10       | 1.17          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 20       | 1.17          |
| (2,524)  | 1:137:B:LEU:HD11  | 1:137:B:LEU:HB2   | 6        | 1.17          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG13 | 3        | 1.17          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG12 | 10       | 1.17          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 15       | 1.16          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 11       | 1.16          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 1        | 1.16          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 16       | 1.16          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 1        | 1.16          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 7        | 1.16          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 15       | 1.16          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 6        | 1.16          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 10       | 1.16          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 1        | 1.16          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 11       | 1.16          |
| (2,524)  | 1:137:B:LEU:HD12  | 1:137:B:LEU:HB2   | 2        | 1.16          |
| (2,524)  | 1:137:B:LEU:HD12  | 1:137:B:LEU:HB2   | 9        | 1.16          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG13 | 5        | 1.16          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 7        | 1.16          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 8        | 1.16          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG12 | 17       | 1.16          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 3        | 1.15          |
| (2,1565) | 2:1794:A:LYS:HB3  | 2:1795:A:HIS:HB2  | 11       | 1.15          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 6        | 1.15          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 7        | 1.15          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 20       | 1.15          |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD2   | 9        | 1.15          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 7        | 1.15          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 18       | 1.15          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 12       | 1.14          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 2        | 1.14          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 9        | 1.14          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 10       | 1.14          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 12       | 1.14          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 20       | 1.14          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 11       | 1.14          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 18       | 1.14          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 19       | 1.14          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 1        | 1.14          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 10       | 1.14          |
| (2,561)  | 1:119:B:VAL:HG21  | 1:118:B:ASP:HB3   | 16       | 1.14          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 10       | 1.14          |
| (2,524)  | 1:137:B:LEU:HD13  | 1:137:B:LEU:HB2   | 8        | 1.14          |
| (2,524)  | 1:137:B:LEU:HD12  | 1:137:B:LEU:HB2   | 18       | 1.14          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 1        | 1.13          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 20       | 1.13          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 4        | 1.13          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 1        | 1.13          |
| (2,1507) | 2:1735:A:ILE:HA   | 2:1739:A:ILE:HG12 | 13       | 1.13          |
| (2,1148) | 2:1788:A:LEU:HD21 | 1:130:B:TYR:HD2   | 6        | 1.13          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 12       | 1.13          |
| (2,802)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:HA   | 17       | 1.13          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 10       | 1.13          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 14       | 1.13          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 18       | 1.13          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 5        | 1.13          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 9        | 1.13          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 16       | 1.13          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 17       | 1.12          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 13       | 1.12          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 13       | 1.12          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 6        | 1.12          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 17       | 1.12          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 3        | 1.12          |
| (2,1135) | 2:1765:A:VAL:HG12 | 2:1804:A:PRO:HG2  | 14       | 1.12          |
| (2,1133) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:HG2  | 5        | 1.12          |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 10       | 1.12          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 4        | 1.12          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 8        | 1.12          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG12 | 6        | 1.12          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 16       | 1.11          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 8        | 1.11          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2  | 6        | 1.11          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 19       | 1.11          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 4        | 1.11          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 6        | 1.11          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 2        | 1.11          |
| (2,676)  | 1:132:B:GLU:HG2   | 1:135:B:LEU:HB2   | 18       | 1.11          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 19       | 1.11          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG11 | 16       | 1.11          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 14       | 1.1           |
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3  | 11       | 1.1           |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 14       | 1.1           |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 3        | 1.1           |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 9        | 1.1           |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 12       | 1.1           |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 17       | 1.1           |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 16       | 1.1           |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 4        | 1.1           |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 3        | 1.09          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 4        | 1.09          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 18       | 1.09          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 12       | 1.09          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 8        | 1.09          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 13       | 1.09          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 14       | 1.09          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD11 | 20       | 1.09          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,884)  | 2:1759:A:GLN:HA   | 2:1762:A:LYS:HB3  | 11       | 1.09          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 16       | 1.09          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 13       | 1.09          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 13       | 1.08          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 5        | 1.08          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 6        | 1.08          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 14       | 1.08          |
| (2,1148) | 2:1788:A:LEU:HD21 | 1:130:B:TYR:HD2   | 19       | 1.08          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 2        | 1.08          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 8        | 1.08          |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA    | 8        | 1.08          |
| (2,1704) | 2:1801:A:CYS:HB2  | 2:1807:A:LEU:H    | 17       | 1.07          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 9        | 1.07          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 13       | 1.07          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 12       | 1.07          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 6        | 1.07          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 19       | 1.07          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 13       | 1.07          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 6        | 1.07          |
| (2,676)  | 1:132:B:GLU:HG2   | 1:135:B:LEU:HB2   | 7        | 1.07          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 8        | 1.07          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 16       | 1.07          |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA    | 11       | 1.07          |
| (2,285)  | 2:1803:A:VAL:H    | 2:1743:A:VAL:HG13 | 2        | 1.07          |
| (2,192)  | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG22  | 7        | 1.07          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD12  | 15       | 1.06          |
| (2,1687) | 2:1745:A:ALA:HB2  | 2:1762:A:LYS:HB3  | 2        | 1.06          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 2        | 1.06          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 3        | 1.06          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 8        | 1.06          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 1        | 1.06          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 3        | 1.06          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 16       | 1.06          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 10       | 1.06          |
| (2,1176) | 2:1755:A:LEU:HD11 | 2:1756:A:PRO:HD3  | 1        | 1.06          |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 4        | 1.06          |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 10       | 1.06          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 8        | 1.06          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 18       | 1.06          |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD11  | 14       | 1.06          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 1        | 1.06          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 11       | 1.05          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3  | 10       | 1.05          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 12       | 1.05          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 17       | 1.05          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB1  | 1        | 1.05          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 14       | 1.05          |
| (2,1039) | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HB2  | 18       | 1.05          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 11       | 1.05          |
| (2,933)  | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE2  | 13       | 1.05          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 7        | 1.05          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 14       | 1.05          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 15       | 1.05          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 4        | 1.05          |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA    | 19       | 1.05          |
| (2,488)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HG13  | 13       | 1.05          |
| (2,1709) | 2:1741:A:SER:HB3  | 2:1742:A:LEU:HB2  | 20       | 1.04          |
| (2,1687) | 2:1745:A:ALA:HB2  | 2:1762:A:LYS:HB3  | 1        | 1.04          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 2        | 1.04          |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 2        | 1.04          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 4        | 1.04          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 8        | 1.04          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 18       | 1.04          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD12 | 19       | 1.04          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 4        | 1.04          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 13       | 1.04          |
| (2,679)  | 1:135:B:LEU:HD11  | 1:132:B:GLU:HA    | 2        | 1.04          |
| (2,679)  | 1:135:B:LEU:HD12  | 1:132:B:GLU:HA    | 18       | 1.04          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 17       | 1.04          |
| (2,677)  | 1:132:B:GLU:HG2   | 1:131:B:ASN:H     | 20       | 1.04          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 6        | 1.04          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 7        | 1.04          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 11       | 1.04          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H     | 11       | 1.04          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3  | 4        | 1.03          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H    | 4        | 1.03          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H    | 18       | 1.03          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 7        | 1.03          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA   | 10       | 1.03          |
| (2,1181) | 2:1758:A:CYS:HB2  | 2:1755:A:LEU:HB2  | 10       | 1.03          |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 8        | 1.03          |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 17       | 1.03          |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 14       | 1.03          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD13 | 13       | 1.03          |

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| Key      | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|----------|-------------------|------------------|----------|---------------|
| (2,850)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB3 | 10       | 1.03          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H   | 3        | 1.03          |
| (2,679)  | 1:135:B:LEU:HD11  | 1:132:B:GLU:HA   | 15       | 1.03          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3  | 3        | 1.03          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H    | 19       | 1.03          |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA   | 2        | 1.03          |
| (2,1687) | 2:1745:A:ALA:HB2  | 2:1762:A:LYS:HB3 | 10       | 1.02          |
| (2,1687) | 2:1745:A:ALA:HB1  | 2:1762:A:LYS:HB3 | 14       | 1.02          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 15       | 1.02          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H   | 11       | 1.02          |
| (2,1409) | 2:1804:A:PRO:HG2  | 2:1765:A:VAL:HA  | 4        | 1.02          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3 | 8        | 1.02          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3 | 19       | 1.02          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA  | 19       | 1.02          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H   | 4        | 1.02          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 6        | 1.01          |
| (2,1687) | 2:1745:A:ALA:HB2  | 2:1762:A:LYS:HB3 | 7        | 1.01          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA  | 6        | 1.01          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 18       | 1.01          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 10       | 1.01          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 18       | 1.01          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 20       | 1.01          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3  | 17       | 1.01          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD11 | 9        | 1.01          |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H   | 15       | 1.01          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 3        | 1.0           |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 8        | 1.0           |
| (2,1687) | 2:1745:A:ALA:HB1  | 2:1762:A:LYS:HB3 | 17       | 1.0           |
| (2,1687) | 2:1745:A:ALA:HB1  | 2:1762:A:LYS:HB3 | 19       | 1.0           |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA  | 2        | 1.0           |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 4        | 1.0           |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 16       | 1.0           |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3 | 9        | 1.0           |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 11       | 1.0           |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3 | 12       | 1.0           |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3 | 16       | 1.0           |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3 | 2        | 1.0           |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3 | 20       | 1.0           |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB1 | 12       | 1.0           |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD2  | 2        | 1.0           |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD2  | 16       | 1.0           |
| (2,1027) | 2:1742:A:LEU:HD22 | 2:1803:A:VAL:HA  | 5        | 1.0           |

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| Key      | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|----------|-------------------|------------------|----------|---------------|
| (2,1027) | 2:1742:A:LEU:HD22 | 2:1803:A:VAL:HA  | 6        | 1.0           |
| (2,1027) | 2:1742:A:LEU:HD22 | 2:1803:A:VAL:HA  | 8        | 1.0           |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3  | 12       | 1.0           |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H   | 14       | 1.0           |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 11       | 0.99          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 20       | 0.99          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 9        | 0.99          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H   | 8        | 0.99          |
| (2,1396) | 2:1793:A:ALA:HB3  | 2:1796:A:CYS:HB3 | 2        | 0.99          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 4        | 0.99          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 14       | 0.99          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3 | 18       | 0.99          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2 | 15       | 0.99          |
| (2,804)  | 2:1731:A:ARG:HD2  | 2:1732:A:ARG:HA  | 14       | 0.99          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA  | 5        | 0.99          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA  | 16       | 0.99          |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H   | 1        | 0.99          |
| (2,1687) | 2:1745:A:ALA:HB2  | 2:1762:A:LYS:HB3 | 12       | 0.98          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 18       | 0.98          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 8        | 0.98          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 9        | 0.98          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 5        | 0.98          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 19       | 0.98          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3 | 11       | 0.98          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB1 | 10       | 0.98          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB3 | 14       | 0.98          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA  | 11       | 0.98          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 1        | 0.98          |
| (2,1027) | 2:1742:A:LEU:HD22 | 2:1803:A:VAL:HA  | 2        | 0.98          |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA  | 3        | 0.98          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 12       | 0.98          |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA  | 15       | 0.98          |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA  | 19       | 0.98          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2 | 20       | 0.98          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 8        | 0.98          |
| (2,679)  | 1:135:B:LEU:HD13  | 1:132:B:GLU:HA   | 7        | 0.98          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3  | 13       | 0.98          |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA   | 13       | 0.98          |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H   | 4        | 0.98          |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H   | 17       | 0.98          |
| (2,1687) | 2:1745:A:ALA:HB1  | 2:1762:A:LYS:HB3 | 9        | 0.97          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 13       | 0.97          |

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| Key      | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|----------|-------------------|------------------|----------|---------------|
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 3        | 0.97          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 7        | 0.97          |
| (2,1557) | 2:1791:A:TYR:HB2  | 2:1790:A:ALA:H   | 14       | 0.97          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2 | 11       | 0.97          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2 | 20       | 0.97          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA  | 3        | 0.97          |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD1  | 15       | 0.97          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 10       | 0.97          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 16       | 0.97          |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA  | 18       | 0.97          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 3        | 0.97          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 2        | 0.97          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3  | 9        | 0.97          |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA   | 1        | 0.97          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 5        | 0.96          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 15       | 0.96          |
| (2,1687) | 2:1745:A:ALA:HB3  | 2:1762:A:LYS:HB3 | 16       | 0.96          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA  | 1        | 0.96          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA  | 14       | 0.96          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 5        | 0.96          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 19       | 0.96          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3 | 11       | 0.96          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2 | 16       | 0.96          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2 | 5        | 0.96          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2 | 7        | 0.96          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2 | 9        | 0.96          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2 | 20       | 0.96          |
| (2,1027) | 2:1742:A:LEU:HD22 | 2:1803:A:VAL:HA  | 9        | 0.96          |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA  | 17       | 0.96          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 16       | 0.96          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 14       | 0.95          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2 | 16       | 0.95          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2 | 13       | 0.95          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB3 | 17       | 0.95          |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB1 | 7        | 0.95          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2 | 2        | 0.95          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2 | 11       | 0.95          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2 | 13       | 0.95          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 7        | 0.95          |
| (2,1027) | 2:1742:A:LEU:HD23 | 2:1803:A:VAL:HA  | 11       | 0.95          |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA  | 13       | 0.95          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2 | 13       | 0.95          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 12       | 0.95          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 17       | 0.95          |
| (2,666)  | 1:120:B:ILE:HD13  | 1:117:B:ASP:HB3   | 17       | 0.95          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 20       | 0.94          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 11       | 0.94          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 2        | 0.94          |
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3  | 16       | 0.94          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2  | 3        | 0.94          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 12       | 0.94          |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB3  | 17       | 0.94          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 16       | 0.94          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 18       | 0.94          |
| (2,1027) | 2:1742:A:LEU:HD21 | 2:1803:A:VAL:HA   | 20       | 0.94          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 4        | 0.94          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 10       | 0.94          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 16       | 0.94          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD12 | 3        | 0.94          |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H    | 3        | 0.94          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 20       | 0.93          |
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 3        | 0.93          |
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 8        | 0.93          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 17       | 0.93          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 18       | 0.93          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2  | 15       | 0.93          |
| (2,1186) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD2  | 5        | 0.93          |
| (2,1186) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD2  | 12       | 0.93          |
| (2,1120) | 2:1739:A:ILE:HG22 | 2:1792:A:HIS:HB3  | 8        | 0.93          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 2        | 0.93          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 6        | 0.93          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 15       | 0.93          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA   | 11       | 0.93          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 2        | 0.92          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 13       | 0.92          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 17       | 0.92          |
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 17       | 0.92          |
| (2,1365) | 2:1734:A:SER:HA   | 2:1737:A:ARG:HB3  | 15       | 0.92          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 20       | 0.92          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 1        | 0.92          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 1        | 0.92          |
| (2,1186) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD2  | 6        | 0.92          |
| (2,1186) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD2  | 8        | 0.92          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 15       | 0.92          |

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| Key      | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|----------|-------------------|------------------|----------|---------------|
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 17       | 0.92          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 3        | 0.92          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 13       | 0.92          |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H    | 7        | 0.92          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H   | 12       | 0.91          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3 | 18       | 0.91          |
| (2,1524) | 2:1766:A:GLN:HG2  | 2:1766:A:GLN:H   | 15       | 0.91          |
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD1 | 3        | 0.91          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2 | 12       | 0.91          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2 | 8        | 0.91          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2 | 18       | 0.91          |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB3 | 18       | 0.91          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2 | 3        | 0.91          |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD1  | 1        | 0.91          |
| (2,1011) | 2:1807:A:LEU:HD13 | 2:1807:A:LEU:HB2 | 8        | 0.91          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 12       | 0.91          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 19       | 0.91          |
| (2,759)  | 2:1762:A:LYS:HD2  | 2:1745:A:ALA:HA  | 20       | 0.91          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 18       | 0.91          |
| (2,676)  | 1:132:B:GLU:HG2   | 1:135:B:LEU:HB2  | 2        | 0.91          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3  | 2        | 0.91          |
| (2,1396) | 2:1793:A:ALA:HB3  | 2:1796:A:CYS:HB3 | 6        | 0.9           |
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3 | 12       | 0.9           |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB2 | 5        | 0.9           |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2 | 1        | 0.9           |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2 | 16       | 0.9           |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB2 | 2        | 0.9           |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 5        | 0.9           |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 9        | 0.9           |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3 | 15       | 0.9           |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H   | 8        | 0.9           |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H   | 12       | 0.9           |
| (2,851)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB2 | 16       | 0.9           |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H   | 17       | 0.9           |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3  | 20       | 0.9           |
| (2,665)  | 1:119:B:VAL:HG11  | 1:120:B:ILE:HG13 | 3        | 0.9           |
| (2,527)  | 1:133:B:GLU:HG3   | 1:132:B:GLU:H    | 17       | 0.9           |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H    | 19       | 0.9           |
| (2,138)  | 2:1783:A:LYS:HD3  | 2:1783:A:LYS:H   | 8        | 0.9           |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H   | 11       | 0.89          |
| (2,1563) | 2:1781:A:ILE:HB   | 2:1780:A:PRO:HD3 | 17       | 0.89          |
| (2,1554) | 2:1735:A:ILE:HD11 | 2:1791:A:TYR:HE1 | 14       | 0.89          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 13       | 0.89          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 3        | 0.89          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 18       | 0.89          |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB2  | 10       | 0.89          |
| (2,1148) | 2:1788:A:LEU:HD21 | 1:130:B:TYR:HD1   | 3        | 0.89          |
| (2,1039) | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HB2  | 19       | 0.89          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 16       | 0.89          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 7        | 0.89          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 20       | 0.89          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 11       | 0.89          |
| (2,851)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB2  | 3        | 0.89          |
| (2,636)  | 1:135:B:LEU:HD22  | 1:132:B:GLU:HB2   | 2        | 0.89          |
| (2,491)  | 1:122:B:ASP:HB2   | 1:123:B:ILE:HA    | 18       | 0.89          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 10       | 0.88          |
| (2,1554) | 2:1735:A:ILE:HD11 | 2:1791:A:TYR:HE2  | 1        | 0.88          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 15       | 0.88          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 4        | 0.88          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 17       | 0.88          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB3  | 9        | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 2        | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 7        | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 9        | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 11       | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 13       | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 16       | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 18       | 0.88          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 20       | 0.88          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 6        | 0.88          |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB1  | 13       | 0.88          |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 1        | 0.88          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 11       | 0.88          |
| (2,1030) | 2:1807:A:LEU:HD11 | 2:1801:A:CYS:HB2  | 11       | 0.88          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 1        | 0.88          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 13       | 0.88          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 6        | 0.88          |
| (2,851)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB2  | 2        | 0.88          |
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 12       | 0.88          |
| (2,233)  | 2:1732:A:ARG:H    | 2:1731:A:ARG:HG3  | 18       | 0.88          |
| (2,1693) | 2:1755:A:LEU:HD11 | 2:1754:A:SER:HB2  | 3        | 0.87          |
| (2,1572) | 2:1809:A:ILE:HD11 | 2:1805:A:PHE:HD2  | 5        | 0.87          |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE2  | 9        | 0.87          |
| (2,1451) | 2:1789:A:ALA:HB1  | 2:1805:A:PHE:HD1  | 13       | 0.87          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 10       | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 2        | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 4        | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 5        | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD12 | 2:1742:A:LEU:HB3  | 6        | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 8        | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 9        | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 10       | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 12       | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 16       | 0.87          |
| (2,1361) | 2:1742:A:LEU:HD12 | 2:1742:A:LEU:HB3  | 18       | 0.87          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 8        | 0.87          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB3  | 19       | 0.87          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 5        | 0.87          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 6        | 0.87          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 10       | 0.87          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 13       | 0.87          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 7        | 0.87          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 14       | 0.87          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 5        | 0.87          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 6        | 0.87          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 7        | 0.87          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 8        | 0.87          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 20       | 0.87          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 11       | 0.87          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 14       | 0.87          |
| (2,851)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB2  | 1        | 0.87          |
| (2,465)  | 1:137:B:LEU:HD21  | 1:138:B:MET:H     | 17       | 0.87          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 19       | 0.87          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 9        | 0.86          |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE1  | 10       | 0.86          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 7        | 0.86          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 9        | 0.86          |
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3  | 18       | 0.86          |
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3  | 20       | 0.86          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 1        | 0.86          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 3        | 0.86          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 7        | 0.86          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 11       | 0.86          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 13       | 0.86          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 14       | 0.86          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 15       | 0.86          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1361) | 2:1742:A:LEU:HD12 | 2:1742:A:LEU:HB3  | 17       | 0.86          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 2        | 0.86          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 9        | 0.86          |
| (2,1120) | 2:1739:A:ILE:HG22 | 2:1792:A:HIS:HB3  | 15       | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 1        | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 3        | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 9        | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 10       | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 13       | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 14       | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 15       | 0.86          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 18       | 0.86          |
| (2,851)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB2  | 9        | 0.86          |
| (2,851)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB2  | 10       | 0.86          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG22  | 4        | 0.86          |
| (2,560)  | 1:134:B:ILE:HD13  | 1:131:B:ASN:HD22  | 4        | 0.86          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 13       | 0.86          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 18       | 0.86          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 20       | 0.86          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 20       | 0.85          |
| (2,1515) | 2:1764:A:VAL:HG12 | 2:1761:A:MET:HG2  | 5        | 0.85          |
| (2,1361) | 2:1742:A:LEU:HD11 | 2:1742:A:LEU:HB3  | 19       | 0.85          |
| (2,1361) | 2:1742:A:LEU:HD13 | 2:1742:A:LEU:HB3  | 20       | 0.85          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 7        | 0.85          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 16       | 0.85          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 5        | 0.85          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 18       | 0.85          |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB1  | 14       | 0.85          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 2        | 0.85          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 4        | 0.85          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 12       | 0.85          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 19       | 0.85          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 2        | 0.85          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 5        | 0.85          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 7        | 0.85          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 15       | 0.85          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 2        | 0.84          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 2        | 0.84          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 7        | 0.84          |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE2  | 15       | 0.84          |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE1  | 19       | 0.84          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 20       | 0.84          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3  | 4        | 0.84          |
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 9        | 0.84          |
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 14       | 0.84          |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB2  | 5        | 0.84          |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB3  | 16       | 0.84          |
| (2,1120) | 2:1739:A:ILE:HG22 | 2:1792:A:HIS:HB3  | 3        | 0.84          |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 18       | 0.84          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 16       | 0.84          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 6        | 0.84          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 10       | 0.84          |
| (2,671)  | 1:126:B:LEU:HG    | 1:122:B:ASP:HB2   | 18       | 0.84          |
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 1        | 0.84          |
| (2,465)  | 1:137:B:LEU:HD23  | 1:138:B:MET:H     | 11       | 0.84          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 7        | 0.84          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 9        | 0.84          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 16       | 0.84          |
| (2,1704) | 2:1801:A:CYS:HB2  | 2:1807:A:LEU:H    | 11       | 0.83          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 5        | 0.83          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 6        | 0.83          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 9        | 0.83          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 7        | 0.83          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 17       | 0.83          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG12 | 14       | 0.83          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 18       | 0.83          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 1        | 0.83          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 3        | 0.83          |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB2  | 20       | 0.83          |
| (2,1039) | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HB2  | 14       | 0.83          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 18       | 0.83          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 3        | 0.83          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 11       | 0.83          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 1        | 0.82          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 14       | 0.82          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 1        | 0.82          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 15       | 0.82          |
| (2,1554) | 2:1735:A:ILE:HD11 | 2:1791:A:TYR:HE2  | 7        | 0.82          |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE1  | 8        | 0.82          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 10       | 0.82          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 15       | 0.82          |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB2  | 1        | 0.82          |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB3  | 11       | 0.82          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 19       | 0.82          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 8        | 0.82          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 16       | 0.82          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 13       | 0.82          |
| (2,851)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB2  | 19       | 0.82          |
| (2,560)  | 1:134:B:ILE:HD12  | 1:131:B:ASN:HD22  | 3        | 0.82          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 9        | 0.82          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 12       | 0.82          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 20       | 0.82          |
| (2,1704) | 2:1801:A:CYS:HB2  | 2:1807:A:LEU:H    | 4        | 0.81          |
| (2,1693) | 2:1755:A:LEU:HD12 | 2:1754:A:SER:HB2  | 9        | 0.81          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 8        | 0.81          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 15       | 0.81          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 18       | 0.81          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG13 | 2        | 0.81          |
| (2,1595) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HE22 | 7        | 0.81          |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE1  | 5        | 0.81          |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE1  | 18       | 0.81          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 19       | 0.81          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 3        | 0.81          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 3        | 0.81          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 11       | 0.81          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 3        | 0.81          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 17       | 0.81          |
| (2,1184) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD3  | 13       | 0.81          |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD1   | 7        | 0.81          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 13       | 0.81          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 2        | 0.81          |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD23 | 5        | 0.81          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 8        | 0.81          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 9        | 0.81          |
| (2,853)  | 2:1807:A:LEU:HD21 | 2:1807:A:LEU:H    | 19       | 0.81          |
| (2,851)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB2  | 7        | 0.81          |
| (2,851)  | 2:1807:A:LEU:HD22 | 2:1801:A:CYS:HB2  | 14       | 0.81          |
| (2,850)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB3  | 20       | 0.81          |
| (2,672)  | 1:129:B:SER:HA    | 1:132:B:GLU:HG2   | 18       | 0.81          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB1  | 11       | 0.81          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 1        | 0.81          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 10       | 0.81          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 12       | 0.81          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 14       | 0.81          |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 17       | 0.81          |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 15       | 0.8           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 5        | 0.8           |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 6        | 0.8           |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 1        | 0.8           |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 4        | 0.8           |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE2  | 2        | 0.8           |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 4        | 0.8           |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 8        | 0.8           |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 15       | 0.8           |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 18       | 0.8           |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB3  | 6        | 0.8           |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB1  | 12       | 0.8           |
| (2,1120) | 2:1739:A:ILE:HG22 | 2:1792:A:HIS:HB3  | 5        | 0.8           |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 6        | 0.8           |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 14       | 0.8           |
| (2,1052) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HE2  | 3        | 0.8           |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 16       | 0.8           |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 4        | 0.8           |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 6        | 0.8           |
| (2,53)   | 2:1755:A:LEU:HB2  | 2:1755:A:LEU:H    | 8        | 0.8           |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 5        | 0.79          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 12       | 0.79          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 13       | 0.79          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 16       | 0.79          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 8        | 0.79          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 9        | 0.79          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG13 | 13       | 0.79          |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE2  | 6        | 0.79          |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE2  | 17       | 0.79          |
| (2,1432) | 2:1783:A:LYS:HB2  | 2:1783:A:LYS:HE2  | 1        | 0.79          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 5        | 0.79          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 7        | 0.79          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 11       | 0.79          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 19       | 0.79          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 8        | 0.79          |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB2  | 15       | 0.79          |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 10       | 0.79          |
| (2,1084) | 2:1768:A:THR:HG21 | 2:1781:A:ILE:HG21 | 17       | 0.79          |
| (2,853)  | 2:1807:A:LEU:HD23 | 2:1807:A:LEU:H    | 13       | 0.79          |
| (2,853)  | 2:1807:A:LEU:HD22 | 2:1807:A:LEU:H    | 16       | 0.79          |
| (2,666)  | 1:120:B:ILE:HD12  | 1:117:B:ASP:HB3   | 20       | 0.79          |
| (2,521)  | 1:137:B:LEU:HD12  | 1:137:B:LEU:HA    | 16       | 0.79          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 3        | 0.79          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 16       | 0.79          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB2  | 17       | 0.79          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 19       | 0.78          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG13 | 19       | 0.78          |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE1  | 3        | 0.78          |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE2  | 11       | 0.78          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 4        | 0.78          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 9        | 0.78          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 19       | 0.78          |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB2  | 19       | 0.78          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 9        | 0.78          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE3  | 11       | 0.78          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 17       | 0.78          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 4        | 0.78          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 11       | 0.78          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 16       | 0.78          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 5        | 0.78          |
| (2,853)  | 2:1807:A:LEU:HD23 | 2:1807:A:LEU:H    | 2        | 0.78          |
| (2,853)  | 2:1807:A:LEU:HD21 | 2:1807:A:LEU:H    | 14       | 0.78          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD13  | 14       | 0.78          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 3        | 0.78          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 12       | 0.78          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 14       | 0.78          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 10       | 0.78          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 14       | 0.78          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 10       | 0.78          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB1  | 13       | 0.78          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB2  | 15       | 0.78          |
| (2,1659) | 2:1809:A:ILE:HD11 | 2:1808:A:ASN:HB2  | 2        | 0.77          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 7        | 0.77          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 10       | 0.77          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 10       | 0.77          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 16       | 0.77          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG12 | 17       | 0.77          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 2        | 0.77          |
| (2,1432) | 2:1783:A:LYS:HB2  | 2:1783:A:LYS:HE2  | 3        | 0.77          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 1        | 0.77          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 8        | 0.77          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 14       | 0.77          |
| (2,1244) | 2:1775:A:THR:HG23 | 2:1776:A:ASN:HB2  | 6        | 0.77          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 2        | 0.77          |
| (2,1184) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD3  | 14       | 0.77          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE2  | 3        | 0.77          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE2  | 6        | 0.77          |
| (2,1113) | 2:1737:A:ARG:HB3  | 2:1737:A:ARG:H    | 17       | 0.77          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 5        | 0.77          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 10       | 0.77          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 14       | 0.77          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 15       | 0.77          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 18       | 0.77          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 19       | 0.77          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG21 | 14       | 0.77          |
| (2,853)  | 2:1807:A:LEU:HD23 | 2:1807:A:LEU:H    | 10       | 0.77          |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG13 | 11       | 0.77          |
| (2,657)  | 1:135:B:LEU:HD23  | 1:130:B:TYR:HD2   | 12       | 0.77          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 15       | 0.77          |
| (2,465)  | 1:137:B:LEU:HD21  | 1:138:B:MET:H     | 13       | 0.77          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 1        | 0.77          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 10       | 0.77          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 19       | 0.77          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 12       | 0.77          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 18       | 0.77          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 4        | 0.77          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB1  | 6        | 0.77          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 19       | 0.76          |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 14       | 0.76          |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 3        | 0.76          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 3        | 0.76          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 4        | 0.76          |
| (2,1646) | 2:1736:A:GLN:HG2  | 2:1737:A:ARG:H    | 17       | 0.76          |
| (2,1632) | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:H    | 13       | 0.76          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG12 | 15       | 0.76          |
| (2,1554) | 2:1735:A:ILE:HD11 | 2:1791:A:TYR:HE2  | 20       | 0.76          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 6        | 0.76          |
| (2,1400) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:HG2  | 10       | 0.76          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 16       | 0.76          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 17       | 0.76          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 18       | 0.76          |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB2  | 4        | 0.76          |
| (2,1188) | 2:1803:A:VAL:HG12 | 2:1789:A:ALA:HB2  | 9        | 0.76          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 2        | 0.76          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE2  | 5        | 0.76          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 13       | 0.76          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 19       | 0.76          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE3  | 20       | 0.76          |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 6        | 0.76          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 1        | 0.76          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 3        | 0.76          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 13       | 0.76          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG22 | 10       | 0.76          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 3        | 0.76          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 20       | 0.76          |
| (2,853)  | 2:1807:A:LEU:HD21 | 2:1807:A:LEU:H    | 7        | 0.76          |
| (2,850)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB3  | 4        | 0.76          |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 17       | 0.76          |
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 18       | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 5        | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 6        | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 7        | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 8        | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 11       | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 13       | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 15       | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 16       | 0.76          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 18       | 0.76          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 5        | 0.76          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 11       | 0.76          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 9        | 0.76          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD11  | 2        | 0.75          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 2        | 0.75          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 6        | 0.75          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 11       | 0.75          |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE1  | 13       | 0.75          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 14       | 0.75          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 15       | 0.75          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 7        | 0.75          |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 10       | 0.75          |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 13       | 0.75          |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 19       | 0.75          |
| (2,1432) | 2:1783:A:LYS:HB2  | 2:1783:A:LYS:HE2  | 4        | 0.75          |
| (2,1396) | 2:1793:A:ALA:HB3  | 2:1796:A:CYS:HB3  | 15       | 0.75          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 20       | 0.75          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 3        | 0.75          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 13       | 0.75          |
| (2,1188) | 2:1803:A:VAL:HG13 | 2:1789:A:ALA:HB1  | 3        | 0.75          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 16       | 0.75          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 9        | 0.75          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 12       | 0.75          |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 2        | 0.75          |
| (2,1120) | 2:1739:A:ILE:HG22 | 2:1792:A:HIS:HB3  | 16       | 0.75          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 20       | 0.75          |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD21 | 3        | 0.75          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 2        | 0.75          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 8        | 0.75          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 12       | 0.75          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 4        | 0.75          |
| (2,853)  | 2:1807:A:LEU:HD23 | 2:1807:A:LEU:H    | 9        | 0.75          |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG12 | 20       | 0.75          |
| (2,678)  | 1:134:B:ILE:HG23  | 1:131:B:ASN:HD22  | 2        | 0.75          |
| (2,560)  | 1:134:B:ILE:HD11  | 1:131:B:ASN:HD22  | 15       | 0.75          |
| (2,554)  | 1:124:B:ILE:HD13  | 1:124:B:ILE:HA    | 5        | 0.75          |
| (2,554)  | 1:124:B:ILE:HD11  | 1:124:B:ILE:HA    | 6        | 0.75          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG21  | 14       | 0.75          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 2        | 0.75          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 4        | 0.75          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 9        | 0.75          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 1        | 0.75          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 4        | 0.75          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 17       | 0.75          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB1  | 18       | 0.75          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB2  | 19       | 0.75          |
| (2,1704) | 2:1801:A:CYS:HB2  | 2:1807:A:LEU:H    | 12       | 0.74          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 8        | 0.74          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 15       | 0.74          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 8        | 0.74          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 11       | 0.74          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 1        | 0.74          |
| (2,1452) | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:HB3  | 5        | 0.74          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 12       | 0.74          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 14       | 0.74          |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 15       | 0.74          |
| (2,1452) | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:HB3  | 18       | 0.74          |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD1  | 1        | 0.74          |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 13       | 0.74          |
| (2,1396) | 2:1793:A:ALA:HB3  | 2:1796:A:CYS:HB3  | 7        | 0.74          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 15       | 0.74          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 1        | 0.74          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE2  | 4        | 0.74          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 8        | 0.74          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE3  | 15       | 0.74          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 16       | 0.74          |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 7        | 0.74          |
| (2,1120) | 2:1739:A:ILE:HG22 | 2:1792:A:HIS:HB3  | 17       | 0.74          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 10       | 0.74          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG23 | 5        | 0.74          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG21 | 8        | 0.74          |
| (2,1030) | 2:1807:A:LEU:HD11 | 2:1801:A:CYS:HB2  | 17       | 0.74          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 19       | 0.74          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 10       | 0.74          |
| (2,853)  | 2:1807:A:LEU:HD23 | 2:1807:A:LEU:H    | 1        | 0.74          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 13       | 0.74          |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG11 | 16       | 0.74          |
| (2,674)  | 1:131:B:ASN:HA    | 1:133:B:GLU:HB3   | 5        | 0.74          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 17       | 0.74          |
| (2,364)  | 1:133:B:GLU:H     | 1:133:B:GLU:HB3   | 20       | 0.74          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 16       | 0.74          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 3        | 0.74          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB1  | 14       | 0.74          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD11  | 8        | 0.73          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD12  | 18       | 0.73          |
| (2,1704) | 2:1801:A:CYS:HB2  | 2:1807:A:LEU:H    | 13       | 0.73          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 1        | 0.73          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 2        | 0.73          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 9        | 0.73          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 5        | 0.73          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 9        | 0.73          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG12 | 6        | 0.73          |
| (2,1554) | 2:1735:A:ILE:HD11 | 2:1791:A:TYR:HE2  | 16       | 0.73          |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 3        | 0.73          |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 15       | 0.73          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 6        | 0.73          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 8        | 0.73          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 8        | 0.73          |
| (2,1452) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:HB3  | 9        | 0.73          |
| (2,1452) | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:HB3  | 11       | 0.73          |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 16       | 0.73          |
| (2,1452) | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:HB3  | 20       | 0.73          |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 3        | 0.73          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 12       | 0.73          |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 16       | 0.73          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1210) | 2:1784:A:GLN:HG3  | 2:1788:A:LEU:HD23 | 7        | 0.73          |
| (2,1186) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD2  | 13       | 0.73          |
| (2,1184) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD3  | 4        | 0.73          |
| (2,1184) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD3  | 17       | 0.73          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 5        | 0.73          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 7        | 0.73          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 11       | 0.73          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 13       | 0.73          |
| (2,1148) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HD1   | 12       | 0.73          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 10       | 0.73          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 14       | 0.73          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE3  | 18       | 0.73          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 3        | 0.73          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 7        | 0.73          |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG21 | 9        | 0.73          |
| (2,1084) | 2:1768:A:THR:HG21 | 2:1781:A:ILE:HG22 | 20       | 0.73          |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD21 | 1        | 0.73          |
| (2,1083) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HD21 | 18       | 0.73          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG23  | 19       | 0.73          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 9        | 0.73          |
| (2,763)  | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 19       | 0.73          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD11  | 6        | 0.72          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD13  | 11       | 0.72          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD13  | 12       | 0.72          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD13  | 13       | 0.72          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD12  | 19       | 0.72          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 17       | 0.72          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 14       | 0.72          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 3        | 0.72          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 5        | 0.72          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 6        | 0.72          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 7        | 0.72          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 15       | 0.72          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 16       | 0.72          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 18       | 0.72          |
| (2,1659) | 2:1809:A:ILE:HD12 | 2:1808:A:ASN:HB2  | 17       | 0.72          |
| (2,1659) | 2:1809:A:ILE:HD12 | 2:1808:A:ASN:HB2  | 20       | 0.72          |
| (2,1554) | 2:1735:A:ILE:HD12 | 2:1791:A:TYR:HE2  | 4        | 0.72          |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 4        | 0.72          |
| (2,1452) | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:HB3  | 17       | 0.72          |
| (2,1432) | 2:1783:A:LYS:HB2  | 2:1783:A:LYS:HE2  | 17       | 0.72          |
| (2,1396) | 2:1793:A:ALA:HB3  | 2:1796:A:CYS:HB3  | 19       | 0.72          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 7        | 0.72          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 8        | 0.72          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 19       | 0.72          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 7        | 0.72          |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 2        | 0.72          |
| (2,1184) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD3  | 16       | 0.72          |
| (2,1184) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD3  | 18       | 0.72          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 3        | 0.72          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 19       | 0.72          |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 4        | 0.72          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 9        | 0.72          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 12       | 0.72          |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG21 | 13       | 0.72          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG23 | 15       | 0.72          |
| (2,1030) | 2:1807:A:LEU:HD13 | 2:1801:A:CYS:HB2  | 12       | 0.72          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 14       | 0.72          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 1        | 0.72          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 15       | 0.72          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 1        | 0.72          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB1  | 7        | 0.72          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB2  | 8        | 0.72          |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 18       | 0.72          |
| (2,560)  | 1:134:B:ILE:HD12  | 1:131:B:ASN:HD22  | 8        | 0.72          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 11       | 0.72          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 2        | 0.72          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 1        | 0.72          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB2  | 1        | 0.72          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB2  | 5        | 0.72          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD11  | 5        | 0.71          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD12  | 17       | 0.71          |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 5        | 0.71          |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 17       | 0.71          |
| (2,1659) | 2:1809:A:ILE:HD12 | 2:1808:A:ASN:HB2  | 7        | 0.71          |
| (2,1659) | 2:1809:A:ILE:HD12 | 2:1808:A:ASN:HB2  | 8        | 0.71          |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 11       | 0.71          |
| (2,1659) | 2:1809:A:ILE:HD12 | 2:1808:A:ASN:HB2  | 12       | 0.71          |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 14       | 0.71          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 7        | 0.71          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 10       | 0.71          |
| (2,1554) | 2:1735:A:ILE:HD13 | 2:1791:A:TYR:HE2  | 12       | 0.71          |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 1        | 0.71          |
| (2,1526) | 2:1746:A:ALA:HB3  | 2:1804:A:PRO:HD2  | 12       | 0.71          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD2  | 11       | 0.71          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 2        | 0.71          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 4        | 0.71          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 6        | 0.71          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 12       | 0.71          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 10       | 0.71          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 12       | 0.71          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 19       | 0.71          |
| (2,1188) | 2:1803:A:VAL:HG11 | 2:1789:A:ALA:HB2  | 8        | 0.71          |
| (2,1186) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD2  | 14       | 0.71          |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 7        | 0.71          |
| (2,1184) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD3  | 9        | 0.71          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 6        | 0.71          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 18       | 0.71          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 20       | 0.71          |
| (2,1172) | 2:1807:A:LEU:HA   | 2:1807:A:LEU:HD23 | 8        | 0.71          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 9        | 0.71          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG23 | 4        | 0.71          |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG22 | 7        | 0.71          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 6        | 0.71          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 11       | 0.71          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 3        | 0.71          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 2        | 0.71          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 9        | 0.71          |
| (2,940)  | 2:1766:A:GLN:HA   | 2:1769:A:LYS:HG3  | 14       | 0.71          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 5        | 0.71          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 13       | 0.71          |
| (2,853)  | 2:1807:A:LEU:HD21 | 2:1807:A:LEU:H    | 3        | 0.71          |
| (2,632)  | 1:119:B:VAL:HG21  | 1:119:B:VAL:HA    | 4        | 0.71          |
| (2,554)  | 1:124:B:ILE:HD13  | 1:124:B:ILE:HA    | 16       | 0.71          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 13       | 0.71          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 9        | 0.71          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB2  | 2        | 0.71          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB3  | 16       | 0.71          |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD13  | 4        | 0.7           |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD11  | 10       | 0.7           |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD13  | 20       | 0.7           |
| (2,1736) | 2:1755:A:LEU:HD12 | 2:1744:A:HIS:HD2  | 4        | 0.7           |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 13       | 0.7           |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 14       | 0.7           |
| (2,1671) | 2:1802:A:PRO:HD3  | 2:1802:A:PRO:HB3  | 19       | 0.7           |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG12 | 10       | 0.7           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 9        | 0.7           |
| (2,1551) | 2:1735:A:ILE:HG23 | 2:1791:A:TYR:HB2  | 11       | 0.7           |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 1        | 0.7           |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 8        | 0.7           |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 4        | 0.7           |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 16       | 0.7           |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 10       | 0.7           |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 4        | 0.7           |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 8        | 0.7           |
| (2,1052) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HE2  | 4        | 0.7           |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 6        | 0.7           |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG12 | 10       | 0.7           |
| (2,672)  | 1:129:B:SER:HA    | 1:132:B:GLU:HG2   | 10       | 0.7           |
| (2,671)  | 1:126:B:LEU:HG    | 1:122:B:ASP:HB2   | 1        | 0.7           |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 1        | 0.7           |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 2        | 0.7           |
| (2,632)  | 1:119:B:VAL:HG21  | 1:119:B:VAL:HA    | 11       | 0.7           |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 14       | 0.7           |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 2        | 0.7           |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 15       | 0.7           |
| (3,12)   | 1:123:B:ILE:HA    | 1:123:B:ILE:HD13  | 7        | 0.69          |
| (2,1736) | 2:1755:A:LEU:HD12 | 2:1744:A:HIS:HD2  | 17       | 0.69          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 4        | 0.69          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 10       | 0.69          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG13 | 5        | 0.69          |
| (2,1551) | 2:1735:A:ILE:HG23 | 2:1791:A:TYR:HB2  | 20       | 0.69          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 5        | 0.69          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 12       | 0.69          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 17       | 0.69          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 5        | 0.69          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 19       | 0.69          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 10       | 0.69          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 17       | 0.69          |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 11       | 0.69          |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 19       | 0.69          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 12       | 0.69          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 19       | 0.69          |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD22 | 12       | 0.69          |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD21 | 15       | 0.69          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 13       | 0.69          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 11       | 0.69          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 8        | 0.69          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 11       | 0.69          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 20       | 0.69          |
| (2,853)  | 2:1807:A:LEU:HD22 | 2:1807:A:LEU:H    | 20       | 0.69          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 8        | 0.69          |
| (2,632)  | 1:119:B:VAL:HG21  | 1:119:B:VAL:HA    | 17       | 0.69          |
| (2,632)  | 1:119:B:VAL:HG22  | 1:119:B:VAL:HA    | 19       | 0.69          |
| (2,465)  | 1:137:B:LEU:HD21  | 1:138:B:MET:H     | 14       | 0.69          |
| (2,455)  | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 3        | 0.69          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 6        | 0.69          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 18       | 0.69          |
| (2,1736) | 2:1755:A:LEU:HD11 | 2:1744:A:HIS:HD2  | 12       | 0.68          |
| (2,1708) | 2:1770:A:GLY:HA3  | 2:1769:A:LYS:HB3  | 19       | 0.68          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 16       | 0.68          |
| (2,1659) | 2:1809:A:ILE:HD11 | 2:1808:A:ASN:HB2  | 5        | 0.68          |
| (2,1659) | 2:1809:A:ILE:HD12 | 2:1808:A:ASN:HB2  | 6        | 0.68          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 4        | 0.68          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 5        | 0.68          |
| (2,1547) | 2:1729:A:ASP:HB3  | 2:1730:A:SER:HB3  | 20       | 0.68          |
| (2,1526) | 2:1746:A:ALA:HB3  | 2:1804:A:PRO:HD2  | 6        | 0.68          |
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG22 | 7        | 0.68          |
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD1  | 16       | 0.68          |
| (2,1358) | 2:1742:A:LEU:HD12 | 2:1803:A:VAL:HG11 | 13       | 0.68          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 14       | 0.68          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 18       | 0.68          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 19       | 0.68          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 6        | 0.68          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 14       | 0.68          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 15       | 0.68          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 2        | 0.68          |
| (2,1186) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD2  | 4        | 0.68          |
| (2,1186) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD2  | 9        | 0.68          |
| (2,1186) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD2  | 16       | 0.68          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 14       | 0.68          |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 16       | 0.68          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 3        | 0.68          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 10       | 0.68          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 14       | 0.68          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 11       | 0.68          |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG12 | 19       | 0.68          |
| (2,661)  | 1:111:B:ALA:HB3   | 1:112:B:SER:HB3   | 3        | 0.68          |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 5        | 0.68          |
| (2,632)  | 1:119:B:VAL:HG22  | 1:119:B:VAL:HA    | 6        | 0.68          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 7        | 0.68          |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 16       | 0.68          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 5        | 0.68          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 1        | 0.68          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 12       | 0.68          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 13       | 0.68          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 19       | 0.68          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 8        | 0.68          |
| (2,202)  | 2:1797:A:GLN:H    | 2:1798:A:GLU:HG3  | 19       | 0.68          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 13       | 0.68          |
| (2,109)  | 2:1741:A:SER:H    | 2:1738:A:ALA:HB1  | 8        | 0.68          |
| (2,1736) | 2:1755:A:LEU:HD13 | 2:1744:A:HIS:HD2  | 1        | 0.67          |
| (2,1736) | 2:1755:A:LEU:HD11 | 2:1744:A:HIS:HD2  | 6        | 0.67          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 6        | 0.67          |
| (2,1659) | 2:1809:A:ILE:HD11 | 2:1808:A:ASN:HB2  | 10       | 0.67          |
| (2,1659) | 2:1809:A:ILE:HD11 | 2:1808:A:ASN:HB2  | 19       | 0.67          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 2        | 0.67          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 17       | 0.67          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 20       | 0.67          |
| (2,1396) | 2:1793:A:ALA:HB1  | 2:1796:A:CYS:HB3  | 1        | 0.67          |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 9        | 0.67          |
| (2,1364) | 2:1742:A:LEU:HD11 | 2:1743:A:VAL:H    | 1        | 0.67          |
| (2,1364) | 2:1742:A:LEU:HD11 | 2:1743:A:VAL:H    | 12       | 0.67          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 12       | 0.67          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 7        | 0.67          |
| (2,1186) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD2  | 17       | 0.67          |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 20       | 0.67          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 1        | 0.67          |
| (2,1182) | 2:1758:A:CYS:HB2  | 2:1759:A:GLN:H    | 12       | 0.67          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE3  | 7        | 0.67          |
| (2,1120) | 2:1739:A:ILE:HG21 | 2:1792:A:HIS:HB3  | 20       | 0.67          |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG23 | 6        | 0.67          |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG22 | 19       | 0.67          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 12       | 0.67          |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG22 | 4        | 0.67          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 8        | 0.67          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 2        | 0.67          |
| (2,956)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HB3  | 11       | 0.67          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 16       | 0.67          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 7        | 0.67          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 14       | 0.67          |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG13 | 17       | 0.67          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,632)  | 1:119:B:VAL:HG21  | 1:119:B:VAL:HA    | 12       | 0.67          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 16       | 0.67          |
| (2,1693) | 2:1755:A:LEU:HD11 | 2:1754:A:SER:HB2  | 17       | 0.66          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG13 | 3        | 0.66          |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 2        | 0.66          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 6        | 0.66          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 3        | 0.66          |
| (2,1364) | 2:1742:A:LEU:HD12 | 2:1743:A:VAL:H    | 6        | 0.66          |
| (2,1364) | 2:1742:A:LEU:HD11 | 2:1743:A:VAL:H    | 15       | 0.66          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 16       | 0.66          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 6        | 0.66          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 14       | 0.66          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 14       | 0.66          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 7        | 0.66          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 10       | 0.66          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 17       | 0.66          |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG22 | 17       | 0.66          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 13       | 0.66          |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 12       | 0.66          |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 13       | 0.66          |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 17       | 0.66          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 1        | 0.66          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 2        | 0.66          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 4        | 0.66          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 9        | 0.66          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 16       | 0.66          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 6        | 0.66          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 17       | 0.66          |
| (2,763)  | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 20       | 0.66          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 6        | 0.66          |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 8        | 0.66          |
| (2,632)  | 1:119:B:VAL:HG21  | 1:119:B:VAL:HA    | 9        | 0.66          |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 13       | 0.66          |
| (2,632)  | 1:119:B:VAL:HG22  | 1:119:B:VAL:HA    | 15       | 0.66          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 3        | 0.66          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD11  | 17       | 0.66          |
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 7        | 0.66          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 19       | 0.66          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 7        | 0.66          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 10       | 0.66          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 12       | 0.66          |
| (2,1736) | 2:1755:A:LEU:HD12 | 2:1744:A:HIS:HD2  | 8        | 0.65          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1736) | 2:1755:A:LEU:HD11 | 2:1744:A:HIS:HD2  | 14       | 0.65          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 8        | 0.65          |
| (2,1659) | 2:1809:A:ILE:HD11 | 2:1808:A:ASN:HB2  | 16       | 0.65          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 6        | 0.65          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 14       | 0.65          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 5        | 0.65          |
| (2,1442) | 2:1790:A:ALA:HB2  | 2:1791:A:TYR:HB2  | 4        | 0.65          |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 11       | 0.65          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 17       | 0.65          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 18       | 0.65          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 19       | 0.65          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 6        | 0.65          |
| (2,1364) | 2:1742:A:LEU:HD12 | 2:1743:A:VAL:H    | 4        | 0.65          |
| (2,1364) | 2:1742:A:LEU:HD12 | 2:1743:A:VAL:H    | 8        | 0.65          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 18       | 0.65          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 1        | 0.65          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 8        | 0.65          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 10       | 0.65          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 10       | 0.65          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 15       | 0.65          |
| (2,1186) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD2  | 11       | 0.65          |
| (2,1128) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HE1  | 2        | 0.65          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG23 | 16       | 0.65          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG22 | 18       | 0.65          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 3        | 0.65          |
| (2,973)  | 2:1812:A:LYS:HA   | 2:1812:A:LYS:HG2  | 9        | 0.65          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 9        | 0.65          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 18       | 0.65          |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 2        | 0.65          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 3        | 0.65          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 7        | 0.65          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD13 | 4        | 0.65          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 2        | 0.65          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 10       | 0.65          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 18       | 0.65          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 20       | 0.65          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB1  | 6        | 0.65          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 12       | 0.65          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 18       | 0.65          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 1        | 0.65          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 3        | 0.65          |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG11 | 14       | 0.65          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG11 | 4        | 0.65          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 14       | 0.65          |
| (2,679)  | 1:135:B:LEU:HD12  | 1:132:B:GLU:HA    | 3        | 0.65          |
| (2,666)  | 1:120:B:ILE:HD11  | 1:117:B:ASP:HB3   | 13       | 0.65          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 8        | 0.65          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 14       | 0.65          |
| (2,1736) | 2:1755:A:LEU:HD12 | 2:1744:A:HIS:HD2  | 10       | 0.64          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 7        | 0.64          |
| (2,1664) | 2:1811:A:GLN:HG3  | 2:1811:A:GLN:H    | 7        | 0.64          |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD1  | 9        | 0.64          |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 1        | 0.64          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 5        | 0.64          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 10       | 0.64          |
| (2,1364) | 2:1742:A:LEU:HD11 | 2:1743:A:VAL:H    | 11       | 0.64          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 16       | 0.64          |
| (2,1364) | 2:1742:A:LEU:HD11 | 2:1743:A:VAL:H    | 19       | 0.64          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 4        | 0.64          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 2        | 0.64          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 9        | 0.64          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 11       | 0.64          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 3        | 0.64          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 17       | 0.64          |
| (2,1186) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD2  | 18       | 0.64          |
| (2,1084) | 2:1768:A:THR:HG23 | 2:1781:A:ILE:HG23 | 2        | 0.64          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG23 | 5        | 0.64          |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG21 | 11       | 0.64          |
| (2,973)  | 2:1812:A:LYS:HA   | 2:1812:A:LYS:HG2  | 1        | 0.64          |
| (2,973)  | 2:1812:A:LYS:HA   | 2:1812:A:LYS:HG2  | 10       | 0.64          |
| (2,973)  | 2:1812:A:LYS:HA   | 2:1812:A:LYS:HG2  | 18       | 0.64          |
| (2,853)  | 2:1807:A:LEU:HD22 | 2:1807:A:LEU:H    | 4        | 0.64          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 1        | 0.64          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB2  | 2        | 0.64          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB2  | 19       | 0.64          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB1  | 20       | 0.64          |
| (2,763)  | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 3        | 0.64          |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG13 | 14       | 0.64          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 3        | 0.64          |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 10       | 0.64          |
| (2,632)  | 1:119:B:VAL:HG23  | 1:119:B:VAL:HA    | 20       | 0.64          |
| (2,617)  | 1:137:B:LEU:HD21  | 1:137:B:LEU:HA    | 5        | 0.64          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 4        | 0.64          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 5        | 0.64          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 19       | 0.64          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 3        | 0.64          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 8        | 0.63          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 12       | 0.63          |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 9        | 0.63          |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 6        | 0.63          |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 17       | 0.63          |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 19       | 0.63          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 9        | 0.63          |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD2  | 15       | 0.63          |
| (2,1364) | 2:1742:A:LEU:HD12 | 2:1743:A:VAL:H    | 14       | 0.63          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 20       | 0.63          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 9        | 0.63          |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 12       | 0.63          |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 15       | 0.63          |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 17       | 0.63          |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 18       | 0.63          |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 20       | 0.63          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 1        | 0.63          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 14       | 0.63          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 16       | 0.63          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 20       | 0.63          |
| (2,1186) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD2  | 20       | 0.63          |
| (2,1099) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HD3  | 8        | 0.63          |
| (2,1099) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HD3  | 14       | 0.63          |
| (2,1099) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HD3  | 15       | 0.63          |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG21 | 1        | 0.63          |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD23 | 11       | 0.63          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG22  | 18       | 0.63          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 1        | 0.63          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 17       | 0.63          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 15       | 0.63          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 5        | 0.63          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 11       | 0.63          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB1  | 13       | 0.63          |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG13 | 20       | 0.63          |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG13 | 8        | 0.63          |
| (2,725)  | 2:1746:A:ALA:HB3  | 2:1803:A:VAL:HG11 | 13       | 0.63          |
| (2,669)  | 1:120:B:ILE:HG21  | 1:117:B:ASP:H     | 1        | 0.63          |
| (2,465)  | 1:137:B:LEU:HD21  | 1:138:B:MET:H     | 8        | 0.63          |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 7        | 0.63          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 3        | 0.63          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 11       | 0.63          |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 9        | 0.63          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 12       | 0.62          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 4        | 0.62          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 14       | 0.62          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 19       | 0.62          |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 7        | 0.62          |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 9        | 0.62          |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 16       | 0.62          |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD1  | 2        | 0.62          |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD2  | 4        | 0.62          |
| (2,1396) | 2:1793:A:ALA:HB2  | 2:1796:A:CYS:HB3  | 5        | 0.62          |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 15       | 0.62          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 2        | 0.62          |
| (2,1329) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HB3  | 17       | 0.62          |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 14       | 0.62          |
| (2,1284) | 2:1786:A:ILE:HD12 | 2:1786:A:ILE:HA   | 16       | 0.62          |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 17       | 0.62          |
| (2,1284) | 2:1786:A:ILE:HD12 | 2:1786:A:ILE:HA   | 19       | 0.62          |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 16       | 0.62          |
| (2,1264) | 2:1772:A:LYS:HD3  | 2:1772:A:LYS:HE3  | 19       | 0.62          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 5        | 0.62          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 11       | 0.62          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 15       | 0.62          |
| (2,1184) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD3  | 11       | 0.62          |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD1   | 5        | 0.62          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 16       | 0.62          |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD21 | 2        | 0.62          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 2        | 0.62          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 1        | 0.62          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 20       | 0.62          |
| (2,864)  | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HG2  | 3        | 0.62          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD12 | 20       | 0.62          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 4        | 0.62          |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG12 | 7        | 0.62          |
| (2,579)  | 1:126:B:LEU:HD23  | 1:126:B:LEU:HB3   | 3        | 0.62          |
| (2,579)  | 1:126:B:LEU:HD22  | 1:126:B:LEU:HB3   | 14       | 0.62          |
| (2,464)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:H     | 1        | 0.62          |
| (2,464)  | 1:137:B:LEU:HD21  | 1:137:B:LEU:H     | 12       | 0.62          |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 11       | 0.62          |
| (2,463)  | 1:134:B:ILE:HD11  | 1:134:B:ILE:H     | 19       | 0.62          |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 9        | 0.62          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 6        | 0.62          |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD22 | 13       | 0.61          |
| (2,1693) | 2:1755:A:LEU:HD12 | 2:1754:A:SER:HB2  | 1        | 0.61          |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 4        | 0.61          |
| (2,1652) | 2:1810:A:LYS:HB3  | 2:1807:A:LEU:HA   | 16       | 0.61          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG13 | 11       | 0.61          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 20       | 0.61          |
| (2,1551) | 2:1735:A:ILE:HG23 | 2:1791:A:TYR:HB2  | 12       | 0.61          |
| (2,1501) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HG2  | 13       | 0.61          |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 5        | 0.61          |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 14       | 0.61          |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 20       | 0.61          |
| (2,1451) | 2:1789:A:ALA:HB1  | 2:1805:A:PHE:HD1  | 12       | 0.61          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 4        | 0.61          |
| (2,1442) | 2:1790:A:ALA:HB1  | 2:1791:A:TYR:HB2  | 20       | 0.61          |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 1        | 0.61          |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 6        | 0.61          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 7        | 0.61          |
| (2,1364) | 2:1742:A:LEU:HD13 | 2:1743:A:VAL:H    | 9        | 0.61          |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 6        | 0.61          |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 8        | 0.61          |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 13       | 0.61          |
| (2,1284) | 2:1786:A:ILE:HD12 | 2:1786:A:ILE:HA   | 20       | 0.61          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 6        | 0.61          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 8        | 0.61          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 4        | 0.61          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 17       | 0.61          |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG23 | 5        | 0.61          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 18       | 0.61          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD13 | 9        | 0.61          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 6        | 0.61          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB2  | 10       | 0.61          |
| (2,763)  | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 7        | 0.61          |
| (2,725)  | 2:1746:A:ALA:HB3  | 2:1803:A:VAL:HG11 | 18       | 0.61          |
| (2,579)  | 1:126:B:LEU:HD22  | 1:126:B:LEU:HB3   | 9        | 0.61          |
| (2,464)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:H     | 3        | 0.61          |
| (2,464)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:H     | 13       | 0.61          |
| (2,464)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:H     | 17       | 0.61          |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 1        | 0.61          |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 2        | 0.61          |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 6        | 0.61          |
| (2,277)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HD2  | 2        | 0.61          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1659) | 2:1809:A:ILE:HD11 | 2:1808:A:ASN:HB2  | 18       | 0.6           |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 11       | 0.6           |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 14       | 0.6           |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 17       | 0.6           |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 7        | 0.6           |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 9        | 0.6           |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 13       | 0.6           |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 20       | 0.6           |
| (2,1515) | 2:1764:A:VAL:HG12 | 2:1761:A:MET:HG2  | 18       | 0.6           |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 1        | 0.6           |
| (2,1492) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HD3  | 2        | 0.6           |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 7        | 0.6           |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD11 | 17       | 0.6           |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG12 | 20       | 0.6           |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 4        | 0.6           |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 7        | 0.6           |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 9        | 0.6           |
| (2,1284) | 2:1786:A:ILE:HD12 | 2:1786:A:ILE:HA   | 15       | 0.6           |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 4        | 0.6           |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 10       | 0.6           |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 20       | 0.6           |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 6        | 0.6           |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 18       | 0.6           |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG11 | 6        | 0.6           |
| (2,1146) | 2:1788:A:LEU:HD23 | 2:1735:A:ILE:HA   | 14       | 0.6           |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 4        | 0.6           |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 9        | 0.6           |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 20       | 0.6           |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG21 | 12       | 0.6           |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD13 | 18       | 0.6           |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD11 | 7        | 0.6           |
| (2,893)  | 2:1800:A:LYS:HG2  | 2:1800:A:LYS:HA   | 10       | 0.6           |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 11       | 0.6           |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 17       | 0.6           |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB1  | 16       | 0.6           |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB3  | 17       | 0.6           |
| (2,763)  | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 11       | 0.6           |
| (2,752)  | 2:1785:A:LEU:HD22 | 2:1786:A:ILE:H    | 11       | 0.6           |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG12 | 1        | 0.6           |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 16       | 0.6           |
| (2,669)  | 1:120:B:ILE:HG21  | 1:117:B:ASP:H     | 6        | 0.6           |
| (2,669)  | 1:120:B:ILE:HG22  | 1:117:B:ASP:H     | 19       | 0.6           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,666)  | 1:120:B:ILE:HD12  | 1:117:B:ASP:HB3   | 1        | 0.6           |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 12       | 0.6           |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 14       | 0.6           |
| (2,579)  | 1:126:B:LEU:HD23  | 1:126:B:LEU:HB3   | 1        | 0.6           |
| (2,579)  | 1:126:B:LEU:HD22  | 1:126:B:LEU:HB3   | 16       | 0.6           |
| (2,521)  | 1:137:B:LEU:HD13  | 1:137:B:LEU:HA    | 5        | 0.6           |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG23  | 3        | 0.6           |
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 6        | 0.6           |
| (2,464)  | 1:137:B:LEU:HD21  | 1:137:B:LEU:H     | 19       | 0.6           |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 8        | 0.6           |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 10       | 0.6           |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 15       | 0.6           |
| (2,267)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HG3  | 20       | 0.6           |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 3        | 0.6           |
| (3,12)   | 1:123:B:ILE:HA    | 1:126:B:LEU:HD21  | 9        | 0.59          |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 8        | 0.59          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 18       | 0.59          |
| (2,1693) | 2:1755:A:LEU:HD11 | 2:1754:A:SER:HB2  | 4        | 0.59          |
| (2,1659) | 2:1809:A:ILE:HD13 | 2:1808:A:ASN:HB2  | 13       | 0.59          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 3        | 0.59          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 5        | 0.59          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 6        | 0.59          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 12       | 0.59          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 16       | 0.59          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG21 | 6        | 0.59          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG21 | 10       | 0.59          |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 5        | 0.59          |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 6        | 0.59          |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 7        | 0.59          |
| (2,1501) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HG2  | 12       | 0.59          |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 16       | 0.59          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 15       | 0.59          |
| (2,1346) | 2:1755:A:LEU:HD21 | 2:1758:A:CYS:HB3  | 11       | 0.59          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 3        | 0.59          |
| (2,1230) | 2:1769:A:LYS:HB3  | 2:1769:A:LYS:H    | 13       | 0.59          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 2        | 0.59          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 5        | 0.59          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 17       | 0.59          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 15       | 0.59          |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG21 | 15       | 0.59          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 14       | 0.59          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 4        | 0.59          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 5        | 0.59          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 15       | 0.59          |
| (2,893)  | 2:1800:A:LYS:HG2  | 2:1800:A:LYS:HA   | 5        | 0.59          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 8        | 0.59          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB2  | 3        | 0.59          |
| (2,752)  | 2:1785:A:LEU:HD21 | 2:1786:A:ILE:H    | 12       | 0.59          |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG12 | 11       | 0.59          |
| (2,725)  | 2:1746:A:ALA:HB3  | 2:1803:A:VAL:HG11 | 9        | 0.59          |
| (2,656)  | 1:134:B:ILE:HG23  | 2:1784:A:GLN:HE21 | 14       | 0.59          |
| (2,570)  | 1:120:B:ILE:HG23  | 1:117:B:ASP:HB3   | 3        | 0.59          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 14       | 0.59          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 2        | 0.59          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 4        | 0.59          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 17       | 0.59          |
| (2,484)  | 1:126:B:LEU:HD13  | 1:126:B:LEU:HA    | 19       | 0.59          |
| (2,465)  | 1:137:B:LEU:HD23  | 1:138:B:MET:H     | 2        | 0.59          |
| (2,464)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:H     | 11       | 0.59          |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 4        | 0.59          |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 18       | 0.59          |
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 2        | 0.59          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 18       | 0.59          |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 9        | 0.58          |
| (2,1700) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HG2  | 14       | 0.58          |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 8        | 0.58          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 14       | 0.58          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 18       | 0.58          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 2        | 0.58          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 4        | 0.58          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 7        | 0.58          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 3        | 0.58          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 17       | 0.58          |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 8        | 0.58          |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 4        | 0.58          |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 5        | 0.58          |
| (2,1442) | 2:1790:A:ALA:HB2  | 2:1791:A:TYR:HB2  | 9        | 0.58          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 10       | 0.58          |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 5        | 0.58          |
| (2,1364) | 2:1742:A:LEU:HD12 | 2:1743:A:VAL:H    | 17       | 0.58          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 7        | 0.58          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 9        | 0.58          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 13       | 0.58          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 14       | 0.58          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 15       | 0.58          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 16       | 0.58          |
| (2,1284) | 2:1786:A:ILE:HD12 | 2:1786:A:ILE:HA   | 3        | 0.58          |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 10       | 0.58          |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 18       | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 7        | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 8        | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 9        | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 11       | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 13       | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 14       | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 15       | 0.58          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 16       | 0.58          |
| (2,1150) | 2:1743:A:VAL:HG21 | 2:1803:A:VAL:HG12 | 3        | 0.58          |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD23 | 16       | 0.58          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG23  | 5        | 0.58          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 16       | 0.58          |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG21 | 18       | 0.58          |
| (2,973)  | 2:1812:A:LYS:HA   | 2:1812:A:LYS:HG2  | 17       | 0.58          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 4        | 0.58          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 1        | 0.58          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 7        | 0.58          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 9        | 0.58          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 12       | 0.58          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 15       | 0.58          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 18       | 0.58          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 20       | 0.58          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 2        | 0.58          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 13       | 0.58          |
| (2,893)  | 2:1800:A:LYS:HG2  | 2:1800:A:LYS:HA   | 8        | 0.58          |
| (2,893)  | 2:1800:A:LYS:HG2  | 2:1800:A:LYS:HA   | 13       | 0.58          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 9        | 0.58          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 15       | 0.58          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 18       | 0.58          |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG13 | 13       | 0.58          |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG13 | 16       | 0.58          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 16       | 0.58          |
| (2,632)  | 1:119:B:VAL:HG22  | 1:119:B:VAL:HA    | 3        | 0.58          |
| (2,617)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:HA    | 16       | 0.58          |
| (2,579)  | 1:126:B:LEU:HD21  | 1:126:B:LEU:HB3   | 18       | 0.58          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 20       | 0.58          |
| (2,465)  | 1:137:B:LEU:HD23  | 1:138:B:MET:H     | 15       | 0.58          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 20       | 0.58          |
| (2,464)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:H     | 14       | 0.58          |
| (2,463)  | 1:134:B:ILE:HD12  | 1:134:B:ILE:H     | 6        | 0.58          |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 2        | 0.58          |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 15       | 0.58          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 4        | 0.58          |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD22 | 17       | 0.57          |
| (2,1700) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HG2  | 8        | 0.57          |
| (2,1700) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HG2  | 10       | 0.57          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 2        | 0.57          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 8        | 0.57          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 16       | 0.57          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 18       | 0.57          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 19       | 0.57          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 1        | 0.57          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 1        | 0.57          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 8        | 0.57          |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 19       | 0.57          |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 20       | 0.57          |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 10       | 0.57          |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 17       | 0.57          |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD11 | 8        | 0.57          |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 10       | 0.57          |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 19       | 0.57          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 2        | 0.57          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 8        | 0.57          |
| (2,1319) | 2:1730:A:SER:HB3  | 2:1730:A:SER:HA   | 12       | 0.57          |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 11       | 0.57          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 2        | 0.57          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 16       | 0.57          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 1        | 0.57          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 4        | 0.57          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 12       | 0.57          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 19       | 0.57          |
| (2,1193) | 2:1775:A:THR:HA   | 2:1774:A:LYS:HG3  | 11       | 0.57          |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG22 | 13       | 0.57          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 19       | 0.57          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 5        | 0.57          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 6        | 0.57          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 10       | 0.57          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 13       | 0.57          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 16       | 0.57          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 17       | 0.57          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 19       | 0.57          |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 18       | 0.57          |
| (2,909)  | 2:1759:A:GLN:HB3  | 2:1760:A:LYS:H    | 19       | 0.57          |
| (2,893)  | 2:1800:A:LYS:HG2  | 2:1800:A:LYS:HA   | 19       | 0.57          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 10       | 0.57          |
| (2,795)  | 2:1750:A:ASN:HA   | 2:1751:A:ALA:HB1  | 15       | 0.57          |
| (2,752)  | 2:1785:A:LEU:HD22 | 2:1786:A:ILE:H    | 5        | 0.57          |
| (2,752)  | 2:1785:A:LEU:HD22 | 2:1786:A:ILE:H    | 16       | 0.57          |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG13 | 19       | 0.57          |
| (2,661)  | 1:111:B:ALA:HB3   | 1:112:B:SER:HB3   | 10       | 0.57          |
| (2,484)  | 1:126:B:LEU:HD13  | 1:126:B:LEU:HA    | 6        | 0.57          |
| (2,484)  | 1:126:B:LEU:HD13  | 1:126:B:LEU:HA    | 12       | 0.57          |
| (2,464)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:H     | 7        | 0.57          |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 13       | 0.57          |
| (2,463)  | 1:134:B:ILE:HD12  | 1:134:B:ILE:H     | 14       | 0.57          |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 6        | 0.57          |
| (2,368)  | 1:137:B:LEU:H     | 1:137:B:LEU:HB3   | 20       | 0.57          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB2  | 6        | 0.57          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB2  | 13       | 0.57          |
| (2,99)   | 2:1745:A:ALA:HB2  | 2:1744:A:HIS:H    | 13       | 0.57          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB3  | 7        | 0.57          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 6        | 0.56          |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD23 | 10       | 0.56          |
| (2,1710) | 2:1789:A:ALA:HB2  | 2:1790:A:ALA:HA   | 6        | 0.56          |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 13       | 0.56          |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 19       | 0.56          |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 20       | 0.56          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 14       | 0.56          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 10       | 0.56          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 15       | 0.56          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 9        | 0.56          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 11       | 0.56          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 2        | 0.56          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 5        | 0.56          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 16       | 0.56          |
| (2,1551) | 2:1735:A:ILE:HG23 | 2:1791:A:TYR:HB2  | 7        | 0.56          |
| (2,1501) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HG2  | 1        | 0.56          |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 18       | 0.56          |
| (2,1442) | 2:1790:A:ALA:HB3  | 2:1791:A:TYR:HB2  | 7        | 0.56          |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 14       | 0.56          |
| (2,1385) | 2:1785:A:LEU:HD11 | 2:1768:A:THR:HG23 | 1        | 0.56          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1358) | 2:1742:A:LEU:HD12 | 2:1803:A:VAL:HG12 | 19       | 0.56          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 5        | 0.56          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 9        | 0.56          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 11       | 0.56          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 16       | 0.56          |
| (2,1343) | 2:1755:A:LEU:HD21 | 2:1755:A:LEU:HA   | 20       | 0.56          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 13       | 0.56          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 16       | 0.56          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 10       | 0.56          |
| (2,1209) | 2:1733:A:LEU:HB2  | 2:1733:A:LEU:H    | 20       | 0.56          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 3        | 0.56          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 18       | 0.56          |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG22 | 6        | 0.56          |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG21 | 20       | 0.56          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 16       | 0.56          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 3        | 0.56          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 4        | 0.56          |
| (2,957)  | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 8        | 0.56          |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 10       | 0.56          |
| (2,752)  | 2:1785:A:LEU:HD23 | 2:1786:A:ILE:H    | 2        | 0.56          |
| (2,669)  | 1:120:B:ILE:HG22  | 1:117:B:ASP:H     | 11       | 0.56          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG23  | 8        | 0.56          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 17       | 0.56          |
| (2,530)  | 1:134:B:ILE:HA    | 1:134:B:ILE:HG13  | 18       | 0.56          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 7        | 0.56          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 5        | 0.56          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 13       | 0.56          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 1        | 0.56          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB3  | 1        | 0.56          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB3  | 15       | 0.56          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB3  | 17       | 0.56          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 6        | 0.56          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 20       | 0.56          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 15       | 0.56          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 11       | 0.55          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 20       | 0.55          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 12       | 0.55          |
| (2,1699) | 2:1781:A:ILE:HD11 | 2:1767:A:HIS:HD2  | 14       | 0.55          |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 10       | 0.55          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 10       | 0.55          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 15       | 0.55          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 18       | 0.55          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 11       | 0.55          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG23 | 12       | 0.55          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG22 | 15       | 0.55          |
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG22 | 20       | 0.55          |
| (2,1501) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HG2  | 14       | 0.55          |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 3        | 0.55          |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 5        | 0.55          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 11       | 0.55          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 19       | 0.55          |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 2        | 0.55          |
| (2,1394) | 2:1793:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 13       | 0.55          |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD13 | 16       | 0.55          |
| (2,1385) | 2:1785:A:LEU:HD13 | 2:1768:A:THR:HG22 | 3        | 0.55          |
| (2,1385) | 2:1785:A:LEU:HD13 | 2:1768:A:THR:HG21 | 5        | 0.55          |
| (2,1385) | 2:1785:A:LEU:HD13 | 2:1768:A:THR:HG21 | 16       | 0.55          |
| (2,1364) | 2:1742:A:LEU:HD11 | 2:1743:A:VAL:H    | 13       | 0.55          |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG13 | 11       | 0.55          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD22 | 12       | 0.55          |
| (2,1344) | 2:1755:A:LEU:HD22 | 2:1756:A:PRO:HD3  | 2        | 0.55          |
| (2,1344) | 2:1755:A:LEU:HD22 | 2:1756:A:PRO:HD3  | 15       | 0.55          |
| (2,1344) | 2:1755:A:LEU:HD21 | 2:1756:A:PRO:HD3  | 18       | 0.55          |
| (2,1344) | 2:1755:A:LEU:HD22 | 2:1756:A:PRO:HD3  | 19       | 0.55          |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 2        | 0.55          |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 3        | 0.55          |
| (2,1343) | 2:1755:A:LEU:HD21 | 2:1755:A:LEU:HA   | 7        | 0.55          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 1        | 0.55          |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 2        | 0.55          |
| (2,1284) | 2:1786:A:ILE:HD13 | 2:1786:A:ILE:HA   | 12       | 0.55          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 7        | 0.55          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 6        | 0.55          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG12 | 2        | 0.55          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 10       | 0.55          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG22  | 20       | 0.55          |
| (2,1052) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HE2  | 1        | 0.55          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 5        | 0.55          |
| (2,915)  | 2:1773:A:ARG:HG2  | 2:1773:A:ARG:HD3  | 4        | 0.55          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 11       | 0.55          |
| (2,822)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HG2  | 7        | 0.55          |
| (2,822)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HG2  | 8        | 0.55          |
| (2,822)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HG2  | 17       | 0.55          |
| (2,821)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HB3  | 16       | 0.55          |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG12 | 1        | 0.55          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG13 | 10       | 0.55          |
| (2,726)  | 2:1746:A:ALA:HB1  | 2:1765:A:VAL:HG12 | 18       | 0.55          |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG12 | 2        | 0.55          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 4        | 0.55          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG22  | 1        | 0.55          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG22  | 20       | 0.55          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 8        | 0.55          |
| (2,484)  | 1:126:B:LEU:HD12  | 1:126:B:LEU:HA    | 11       | 0.55          |
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 17       | 0.55          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB2  | 8        | 0.55          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 16       | 0.55          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB3  | 19       | 0.55          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 11       | 0.55          |
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 16       | 0.55          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 3        | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 5        | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 7        | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 8        | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 9        | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 10       | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 12       | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 13       | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 14       | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 15       | 0.54          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 17       | 0.54          |
| (2,1700) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HG2  | 6        | 0.54          |
| (2,1700) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HG2  | 12       | 0.54          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 17       | 0.54          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG11 | 7        | 0.54          |
| (2,1630) | 2:1740:A:GLN:HG3  | 2:1743:A:VAL:HG12 | 20       | 0.54          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 3        | 0.54          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 8        | 0.54          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 13       | 0.54          |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 8        | 0.54          |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 11       | 0.54          |
| (2,1501) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HG2  | 18       | 0.54          |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD11 | 6        | 0.54          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 20       | 0.54          |
| (2,1442) | 2:1790:A:ALA:HB2  | 2:1791:A:TYR:HB2  | 14       | 0.54          |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 20       | 0.54          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD21 | 4        | 0.54          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD21 | 14       | 0.54          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1344) | 2:1755:A:LEU:HD21 | 2:1756:A:PRO:HD3  | 7        | 0.54          |
| (2,1344) | 2:1755:A:LEU:HD23 | 2:1756:A:PRO:HD3  | 16       | 0.54          |
| (2,1344) | 2:1755:A:LEU:HD21 | 2:1756:A:PRO:HD3  | 20       | 0.54          |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 15       | 0.54          |
| (2,1343) | 2:1755:A:LEU:HD21 | 2:1755:A:LEU:HA   | 18       | 0.54          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 8        | 0.54          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 10       | 0.54          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 14       | 0.54          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 5        | 0.54          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 14       | 0.54          |
| (2,1150) | 2:1743:A:VAL:HG23 | 2:1803:A:VAL:HG11 | 16       | 0.54          |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD1   | 13       | 0.54          |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG22 | 8        | 0.54          |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG21 | 9        | 0.54          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 19       | 0.54          |
| (2,915)  | 2:1773:A:ARG:HG2  | 2:1773:A:ARG:HD3  | 13       | 0.54          |
| (2,819)  | 2:1749:A:ARG:HA   | 2:1749:A:ARG:HD3  | 6        | 0.54          |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG12 | 3        | 0.54          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 13       | 0.54          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD13  | 7        | 0.54          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 17       | 0.54          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG22  | 7        | 0.54          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG23  | 8        | 0.54          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 15       | 0.54          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 2        | 0.54          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 3        | 0.54          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 4        | 0.54          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 5        | 0.54          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 19       | 0.54          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 20       | 0.54          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 4        | 0.54          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB3  | 5        | 0.54          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 12       | 0.54          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB2  | 18       | 0.54          |
| (2,120)  | 2:1752:A:ASN:H    | 2:1752:A:ASN:HD22 | 7        | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 3        | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 4        | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 5        | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 7        | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 8        | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 9        | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 10       | 0.54          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 12       | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 13       | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 14       | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 15       | 0.54          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 17       | 0.54          |
| (2,99)   | 2:1745:A:ALA:HB3  | 2:1744:A:HIS:H    | 2        | 0.54          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 9        | 0.54          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 5        | 0.54          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 4        | 0.53          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 4        | 0.53          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 16       | 0.53          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 18       | 0.53          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 19       | 0.53          |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD23 | 11       | 0.53          |
| (2,1700) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HG2  | 17       | 0.53          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 4        | 0.53          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 6        | 0.53          |
| (2,1553) | 2:1781:A:ILE:HG13 | 2:1781:A:ILE:HG21 | 18       | 0.53          |
| (2,1478) | 2:1789:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 11       | 0.53          |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 12       | 0.53          |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG13 | 14       | 0.53          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD22 | 1        | 0.53          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD21 | 6        | 0.53          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD21 | 10       | 0.53          |
| (2,1344) | 2:1755:A:LEU:HD22 | 2:1756:A:PRO:HD3  | 3        | 0.53          |
| (2,1344) | 2:1755:A:LEU:HD23 | 2:1756:A:PRO:HD3  | 13       | 0.53          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 13       | 0.53          |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 19       | 0.53          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 14       | 0.53          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 17       | 0.53          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 13       | 0.53          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 1        | 0.53          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 5        | 0.53          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 12       | 0.53          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 15       | 0.53          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 2        | 0.53          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 6        | 0.53          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 9        | 0.53          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 13       | 0.53          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG13 | 5        | 0.53          |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD2   | 17       | 0.53          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 3        | 0.53          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 15       | 0.53          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG23 | 14       | 0.53          |
| (2,1002) | 2:1738:A:ALA:HB2  | 2:1739:A:ILE:HA   | 14       | 0.53          |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG22 | 3        | 0.53          |
| (2,998)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HG3  | 7        | 0.53          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 1        | 0.53          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 4        | 0.53          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 12       | 0.53          |
| (2,966)  | 2:1739:A:ILE:HD11 | 2:1788:A:LEU:HB2  | 1        | 0.53          |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 3        | 0.53          |
| (2,915)  | 2:1773:A:ARG:HG2  | 2:1773:A:ARG:HD3  | 3        | 0.53          |
| (2,893)  | 2:1800:A:LYS:HG2  | 2:1800:A:LYS:HA   | 20       | 0.53          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 10       | 0.53          |
| (2,802)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:HA   | 2        | 0.53          |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 19       | 0.53          |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG12 | 7        | 0.53          |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG12 | 17       | 0.53          |
| (2,725)  | 2:1746:A:ALA:HB1  | 2:1803:A:VAL:HG13 | 5        | 0.53          |
| (2,725)  | 2:1746:A:ALA:HB2  | 2:1803:A:VAL:HG12 | 15       | 0.53          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 13       | 0.53          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG21  | 11       | 0.53          |
| (2,484)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HA    | 10       | 0.53          |
| (2,465)  | 1:137:B:LEU:HD23  | 1:138:B:MET:H     | 16       | 0.53          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 10       | 0.53          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD11  | 19       | 0.53          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 16       | 0.53          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 1        | 0.53          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 6        | 0.53          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 12       | 0.53          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 15       | 0.53          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 18       | 0.53          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB3  | 2        | 0.53          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 3        | 0.53          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 7        | 0.53          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 9        | 0.53          |
| (2,120)  | 2:1752:A:ASN:H    | 2:1752:A:ASN:HD22 | 2        | 0.53          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 1        | 0.53          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 16       | 0.53          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 18       | 0.53          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 19       | 0.53          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 11       | 0.53          |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 1        | 0.53          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 19       | 0.53          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 1        | 0.53          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 1        | 0.52          |
| (3,13)   | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 2        | 0.52          |
| (2,1699) | 2:1781:A:ILE:HD11 | 2:1767:A:HIS:HD2  | 13       | 0.52          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 5        | 0.52          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 16       | 0.52          |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE1  | 18       | 0.52          |
| (2,1555) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HD1   | 3        | 0.52          |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 2        | 0.52          |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 16       | 0.52          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG23 | 6        | 0.52          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 7        | 0.52          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 14       | 0.52          |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG23 | 1        | 0.52          |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG23 | 3        | 0.52          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD22 | 8        | 0.52          |
| (2,1348) | 2:1755:A:LEU:HB3  | 2:1755:A:LEU:HD23 | 17       | 0.52          |
| (2,1344) | 2:1755:A:LEU:HD23 | 2:1756:A:PRO:HD3  | 5        | 0.52          |
| (2,1344) | 2:1755:A:LEU:HD23 | 2:1756:A:PRO:HD3  | 9        | 0.52          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 12       | 0.52          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 15       | 0.52          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 20       | 0.52          |
| (2,1284) | 2:1786:A:ILE:HD11 | 2:1786:A:ILE:HA   | 1        | 0.52          |
| (2,1284) | 2:1786:A:ILE:HD12 | 2:1786:A:ILE:HA   | 5        | 0.52          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 3        | 0.52          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 17       | 0.52          |
| (2,1244) | 2:1775:A:THR:HG22 | 2:1776:A:ASN:HB2  | 12       | 0.52          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 11       | 0.52          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 20       | 0.52          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 2        | 0.52          |
| (2,1098) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HE2  | 7        | 0.52          |
| (2,1098) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HE2  | 15       | 0.52          |
| (2,1085) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:H    | 7        | 0.52          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG22  | 4        | 0.52          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 10       | 0.52          |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 7        | 0.52          |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 20       | 0.52          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 18       | 0.52          |
| (2,966)  | 2:1739:A:ILE:HD11 | 2:1788:A:LEU:HB2  | 4        | 0.52          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 13       | 0.52          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 4        | 0.52          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 5        | 0.52          |
| (2,819)  | 2:1749:A:ARG:HA   | 2:1749:A:ARG:HD3  | 19       | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 1        | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 2        | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 9        | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 11       | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 12       | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 18       | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 19       | 0.52          |
| (2,800)  | 2:1732:A:ARG:HD3  | 2:1732:A:ARG:HG3  | 20       | 0.52          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 3        | 0.52          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 7        | 0.52          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 8        | 0.52          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 11       | 0.52          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 12       | 0.52          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 19       | 0.52          |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG13 | 3        | 0.52          |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG11 | 5        | 0.52          |
| (2,725)  | 2:1746:A:ALA:HB3  | 2:1803:A:VAL:HG11 | 6        | 0.52          |
| (2,725)  | 2:1746:A:ALA:HB3  | 2:1803:A:VAL:HG13 | 12       | 0.52          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD22 | 2        | 0.52          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 11       | 0.52          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 7        | 0.52          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 8        | 0.52          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 9        | 0.52          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 11       | 0.52          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 16       | 0.52          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 20       | 0.52          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 3        | 0.52          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 5        | 0.52          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 6        | 0.52          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 10       | 0.52          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB2  | 14       | 0.52          |
| (2,120)  | 2:1752:A:ASN:H    | 2:1752:A:ASN:HD22 | 1        | 0.52          |
| (2,106)  | 2:1741:A:SER:HB3  | 2:1741:A:SER:H    | 2        | 0.52          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 5        | 0.52          |
| (2,99)   | 2:1745:A:ALA:HB3  | 2:1744:A:HIS:H    | 7        | 0.52          |
| (2,99)   | 2:1745:A:ALA:HB2  | 2:1744:A:HIS:H    | 9        | 0.52          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 10       | 0.52          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 13       | 0.51          |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD21 | 18       | 0.51          |
| (2,1700) | 2:1755:A:LEU:HD11 | 2:1756:A:PRO:HG2  | 1        | 0.51          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1700) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HG2  | 4        | 0.51          |
| (2,1699) | 2:1781:A:ILE:HD12 | 2:1767:A:HIS:HD2  | 7        | 0.51          |
| (2,1693) | 2:1755:A:LEU:HD13 | 2:1754:A:SER:HB2  | 10       | 0.51          |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 18       | 0.51          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 3        | 0.51          |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 12       | 0.51          |
| (2,1555) | 2:1735:A:ILE:HD13 | 1:130:B:TYR:HD2   | 14       | 0.51          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 4        | 0.51          |
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 10       | 0.51          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 15       | 0.51          |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 3        | 0.51          |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 1        | 0.51          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 5        | 0.51          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 11       | 0.51          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 6        | 0.51          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 6        | 0.51          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 19       | 0.51          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 20       | 0.51          |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 2        | 0.51          |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 5        | 0.51          |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 7        | 0.51          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 12       | 0.51          |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 8        | 0.51          |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 10       | 0.51          |
| (2,1146) | 2:1788:A:LEU:HD23 | 2:1735:A:ILE:HA   | 2        | 0.51          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG23  | 8        | 0.51          |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG22 | 10       | 0.51          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 20       | 0.51          |
| (2,966)  | 2:1739:A:ILE:HD13 | 2:1788:A:LEU:HB2  | 7        | 0.51          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 16       | 0.51          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD12 | 10       | 0.51          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 3        | 0.51          |
| (2,822)  | 2:1749:A:ARG:HD3  | 2:1749:A:ARG:HG2  | 13       | 0.51          |
| (2,819)  | 2:1749:A:ARG:HA   | 2:1749:A:ARG:HD3  | 2        | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 2        | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 4        | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 6        | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 10       | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 13       | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 16       | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 18       | 0.51          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 20       | 0.51          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,750)  | 2:1812:A:LYS:HG2  | 2:1812:A:LYS:H    | 9        | 0.51          |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG11 | 4        | 0.51          |
| (2,726)  | 2:1746:A:ALA:HB1  | 2:1765:A:VAL:HG11 | 9        | 0.51          |
| (2,668)  | 1:120:B:ILE:HD13  | 1:116:B:MET:HA    | 14       | 0.51          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 2        | 0.51          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 4        | 0.51          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 5        | 0.51          |
| (2,558)  | 1:120:B:ILE:HD11  | 1:120:B:ILE:H     | 6        | 0.51          |
| (2,558)  | 1:120:B:ILE:HD11  | 1:120:B:ILE:H     | 13       | 0.51          |
| (2,558)  | 1:120:B:ILE:HD11  | 1:120:B:ILE:H     | 14       | 0.51          |
| (2,558)  | 1:120:B:ILE:HD11  | 1:120:B:ILE:H     | 19       | 0.51          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 4        | 0.51          |
| (2,484)  | 1:126:B:LEU:HD12  | 1:126:B:LEU:HA    | 7        | 0.51          |
| (2,484)  | 1:126:B:LEU:HD12  | 1:126:B:LEU:HA    | 15       | 0.51          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 2        | 0.51          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 5        | 0.51          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD11  | 12       | 0.51          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 13       | 0.51          |
| (2,275)  | 2:1778:A:GLY:H    | 2:1776:A:ASN:HB2  | 18       | 0.51          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 10       | 0.51          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 14       | 0.51          |
| (2,222)  | 2:1763:A:ARG:HB3  | 2:1763:A:ARG:H    | 17       | 0.51          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 3        | 0.51          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 4        | 0.51          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 12       | 0.51          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 14       | 0.51          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 16       | 0.51          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 17       | 0.51          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB2  | 11       | 0.51          |
| (2,125)  | 2:1737:A:ARG:H    | 2:1738:A:ALA:HB1  | 20       | 0.51          |
| (2,99)   | 2:1745:A:ALA:HB3  | 2:1744:A:HIS:H    | 17       | 0.51          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB3  | 13       | 0.51          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB2  | 17       | 0.51          |
| (2,82)   | 2:1764:A:VAL:HG11 | 2:1764:A:VAL:H    | 9        | 0.51          |
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 12       | 0.51          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 11       | 0.51          |
| (2,1699) | 2:1781:A:ILE:HD12 | 2:1767:A:HIS:HD2  | 6        | 0.5           |
| (2,1699) | 2:1781:A:ILE:HD13 | 2:1767:A:HIS:HD2  | 20       | 0.5           |
| (2,1698) | 2:1788:A:LEU:HD21 | 2:1787:A:ALA:H    | 5        | 0.5           |
| (2,1655) | 2:1787:A:ALA:HB2  | 2:1784:A:GLN:HB3  | 9        | 0.5           |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 15       | 0.5           |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 1        | 0.5           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 9        | 0.5           |
| (2,1639) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:H    | 11       | 0.5           |
| (2,1622) | 2:1747:A:GLN:HB3  | 2:1747:A:GLN:HE22 | 1        | 0.5           |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE1  | 15       | 0.5           |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 10       | 0.5           |
| (2,1501) | 2:1781:A:ILE:HD13 | 2:1780:A:PRO:HG2  | 15       | 0.5           |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 17       | 0.5           |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 2        | 0.5           |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 3        | 0.5           |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 15       | 0.5           |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 18       | 0.5           |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD2  | 10       | 0.5           |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 3        | 0.5           |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 9        | 0.5           |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 4        | 0.5           |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD13 | 18       | 0.5           |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG11 | 18       | 0.5           |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 7        | 0.5           |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 19       | 0.5           |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 4        | 0.5           |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 9        | 0.5           |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 11       | 0.5           |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 7        | 0.5           |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 1        | 0.5           |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 3        | 0.5           |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 4        | 0.5           |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 8        | 0.5           |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 10       | 0.5           |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 11       | 0.5           |
| (2,1242) | 2:1772:A:LYS:HG2  | 2:1772:A:LYS:HE3  | 13       | 0.5           |
| (2,1228) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:HA   | 1        | 0.5           |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 3        | 0.5           |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 13       | 0.5           |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 13       | 0.5           |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 6        | 0.5           |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 12       | 0.5           |
| (2,1002) | 2:1738:A:ALA:HB3  | 2:1739:A:ILE:HA   | 2        | 0.5           |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 9        | 0.5           |
| (2,1002) | 2:1738:A:ALA:HB3  | 2:1739:A:ILE:HA   | 17       | 0.5           |
| (2,1002) | 2:1738:A:ALA:HB3  | 2:1739:A:ILE:HA   | 19       | 0.5           |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 9        | 0.5           |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 17       | 0.5           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD13 | 20       | 0.5           |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 12       | 0.5           |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 15       | 0.5           |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 8        | 0.5           |
| (2,819)  | 2:1749:A:ARG:HA   | 2:1749:A:ARG:HD3  | 10       | 0.5           |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 1        | 0.5           |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 14       | 0.5           |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 15       | 0.5           |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 17       | 0.5           |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG12 | 2        | 0.5           |
| (2,666)  | 1:120:B:ILE:HD11  | 1:117:B:ASP:HB3   | 7        | 0.5           |
| (2,666)  | 1:120:B:ILE:HD11  | 1:117:B:ASP:HB3   | 8        | 0.5           |
| (2,661)  | 1:111:B:ALA:HB2   | 1:112:B:SER:HB3   | 14       | 0.5           |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 10       | 0.5           |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 16       | 0.5           |
| (2,463)  | 1:134:B:ILE:HD11  | 1:134:B:ILE:H     | 20       | 0.5           |
| (2,386)  | 1:126:B:LEU:H     | 1:126:B:LEU:HD13  | 18       | 0.5           |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD13  | 11       | 0.5           |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 9        | 0.5           |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 7        | 0.5           |
| (2,249)  | 2:1781:A:ILE:HG22 | 2:1781:A:ILE:H    | 20       | 0.5           |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 11       | 0.5           |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 1        | 0.5           |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 8        | 0.5           |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 11       | 0.5           |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 13       | 0.5           |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 18       | 0.5           |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 19       | 0.5           |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 20       | 0.5           |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 6        | 0.5           |
| (2,99)   | 2:1745:A:ALA:HB2  | 2:1744:A:HIS:H    | 14       | 0.5           |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB2  | 11       | 0.5           |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 20       | 0.5           |
| (2,82)   | 2:1764:A:VAL:HG11 | 2:1764:A:VAL:H    | 5        | 0.5           |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 16       | 0.5           |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 3        | 0.49          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 1        | 0.49          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 3        | 0.49          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 6        | 0.49          |
| (2,1518) | 2:1764:A:VAL:HG11 | 2:1766:A:GLN:H    | 8        | 0.49          |
| (2,1518) | 2:1764:A:VAL:HG11 | 2:1766:A:GLN:H    | 9        | 0.49          |
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 11       | 0.49          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1514) | 2:1764:A:VAL:HG12 | 2:1781:A:ILE:HG22 | 19       | 0.49          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 20       | 0.49          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 12       | 0.49          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 20       | 0.49          |
| (2,1451) | 2:1789:A:ALA:HB1  | 2:1805:A:PHE:HD1  | 14       | 0.49          |
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD2  | 17       | 0.49          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 2        | 0.49          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 11       | 0.49          |
| (2,1415) | 2:1735:A:ILE:HD12 | 2:1735:A:ILE:H    | 1        | 0.49          |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 6        | 0.49          |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 13       | 0.49          |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG23 | 15       | 0.49          |
| (2,1385) | 2:1785:A:LEU:HD11 | 2:1768:A:THR:HG21 | 2        | 0.49          |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG12 | 7        | 0.49          |
| (2,1344) | 2:1755:A:LEU:HD23 | 2:1756:A:PRO:HD3  | 11       | 0.49          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 9        | 0.49          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 10       | 0.49          |
| (2,1244) | 2:1775:A:THR:HG21 | 2:1776:A:ASN:HB2  | 17       | 0.49          |
| (2,1228) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:HA   | 9        | 0.49          |
| (2,1120) | 2:1739:A:ILE:HG23 | 2:1792:A:HIS:HB3  | 12       | 0.49          |
| (2,1098) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HE2  | 17       | 0.49          |
| (2,1084) | 2:1768:A:THR:HG21 | 2:1781:A:ILE:HG21 | 3        | 0.49          |
| (2,1002) | 2:1738:A:ALA:HB3  | 2:1739:A:ILE:HA   | 1        | 0.49          |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 3        | 0.49          |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 10       | 0.49          |
| (2,1002) | 2:1738:A:ALA:HB2  | 2:1739:A:ILE:HA   | 13       | 0.49          |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 16       | 0.49          |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG22 | 1        | 0.49          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 16       | 0.49          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 2        | 0.49          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD13 | 5        | 0.49          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 2        | 0.49          |
| (2,966)  | 2:1739:A:ILE:HD13 | 2:1788:A:LEU:HB2  | 6        | 0.49          |
| (2,966)  | 2:1739:A:ILE:HD13 | 2:1788:A:LEU:HB2  | 11       | 0.49          |
| (2,923)  | 2:1765:A:VAL:HG23 | 2:1745:A:ALA:HB1  | 8        | 0.49          |
| (2,919)  | 2:1765:A:VAL:HG21 | 2:1762:A:LYS:HA   | 6        | 0.49          |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 17       | 0.49          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 5        | 0.49          |
| (2,760)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:H    | 9        | 0.49          |
| (2,750)  | 2:1812:A:LYS:HG2  | 2:1812:A:LYS:H    | 17       | 0.49          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 3        | 0.49          |
| (2,669)  | 1:120:B:ILE:HG21  | 1:117:B:ASP:H     | 16       | 0.49          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 3        | 0.49          |
| (2,465)  | 1:137:B:LEU:HD22  | 1:138:B:MET:H     | 9        | 0.49          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 12       | 0.49          |
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 6        | 0.49          |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 13       | 0.49          |
| (2,249)  | 2:1781:A:ILE:HG22 | 2:1781:A:ILE:H    | 19       | 0.49          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 17       | 0.49          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 2        | 0.49          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 7        | 0.49          |
| (2,99)   | 2:1745:A:ALA:HB2  | 2:1744:A:HIS:H    | 16       | 0.49          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 2        | 0.49          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB2  | 16       | 0.49          |
| (2,82)   | 2:1764:A:VAL:HG11 | 2:1764:A:VAL:H    | 8        | 0.49          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD21 | 12       | 0.49          |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD23 | 12       | 0.48          |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 14       | 0.48          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 2        | 0.48          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 1        | 0.48          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 11       | 0.48          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 13       | 0.48          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 14       | 0.48          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 20       | 0.48          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 11       | 0.48          |
| (2,1604) | 2:1755:A:LEU:HB3  | 2:1758:A:CYS:H    | 19       | 0.48          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 1        | 0.48          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 13       | 0.48          |
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 16       | 0.48          |
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 17       | 0.48          |
| (2,1501) | 2:1781:A:ILE:HD12 | 2:1780:A:PRO:HG2  | 9        | 0.48          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 8        | 0.48          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 12       | 0.48          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 13       | 0.48          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 8        | 0.48          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG23 | 9        | 0.48          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 18       | 0.48          |
| (2,1394) | 2:1793:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 3        | 0.48          |
| (2,1385) | 2:1785:A:LEU:HD11 | 2:1768:A:THR:HG22 | 11       | 0.48          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 11       | 0.48          |
| (2,1317) | 2:1744:A:HIS:HA   | 2:1747:A:GLN:HE22 | 1        | 0.48          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 7        | 0.48          |
| (2,1269) | 2:1727:A:PRO:HB3  | 2:1727:A:PRO:HD2  | 18       | 0.48          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 3        | 0.48          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 13       | 0.48          |
| (2,1228) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:HA   | 18       | 0.48          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 4        | 0.48          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 5        | 0.48          |
| (2,1156) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HE22 | 16       | 0.48          |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 20       | 0.48          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 13       | 0.48          |
| (2,1084) | 2:1768:A:THR:HG22 | 2:1781:A:ILE:HG21 | 12       | 0.48          |
| (2,1002) | 2:1738:A:ALA:HB3  | 2:1739:A:ILE:HA   | 5        | 0.48          |
| (2,1002) | 2:1738:A:ALA:HB2  | 2:1739:A:ILE:HA   | 11       | 0.48          |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 12       | 0.48          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 3        | 0.48          |
| (2,966)  | 2:1739:A:ILE:HD11 | 2:1788:A:LEU:HB2  | 20       | 0.48          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD22 | 16       | 0.48          |
| (2,919)  | 2:1765:A:VAL:HG22 | 2:1762:A:LYS:HA   | 5        | 0.48          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD12 | 14       | 0.48          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 5        | 0.48          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 4        | 0.48          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 12       | 0.48          |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 9        | 0.48          |
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 13       | 0.48          |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 14       | 0.48          |
| (2,726)  | 2:1746:A:ALA:HB3  | 2:1765:A:VAL:HG12 | 15       | 0.48          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 17       | 0.48          |
| (2,668)  | 1:120:B:ILE:HD12  | 1:116:B:MET:HA    | 16       | 0.48          |
| (2,661)  | 1:111:B:ALA:HB1   | 1:112:B:SER:HB3   | 15       | 0.48          |
| (2,661)  | 1:111:B:ALA:HB2   | 1:112:B:SER:HB3   | 19       | 0.48          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 10       | 0.48          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 11       | 0.48          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 16       | 0.48          |
| (2,558)  | 1:120:B:ILE:HD12  | 1:120:B:ILE:H     | 18       | 0.48          |
| (2,538)  | 1:126:B:LEU:HD12  | 1:126:B:LEU:HB2   | 9        | 0.48          |
| (2,538)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HB2   | 14       | 0.48          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 9        | 0.48          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 10       | 0.48          |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG23  | 15       | 0.48          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD13  | 15       | 0.48          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 1        | 0.48          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 14       | 0.48          |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 11       | 0.48          |
| (2,268)  | 2:1773:A:ARG:H    | 2:1773:A:ARG:HD3  | 14       | 0.48          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 5        | 0.48          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB2  | 19       | 0.48          |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 14       | 0.48          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 4        | 0.48          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 10       | 0.48          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 8        | 0.48          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 15       | 0.48          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 18       | 0.48          |
| (2,99)   | 2:1745:A:ALA:HB2  | 2:1744:A:HIS:H    | 19       | 0.48          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB3  | 14       | 0.48          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB2  | 18       | 0.48          |
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 11       | 0.48          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 6        | 0.48          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 2        | 0.48          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 3        | 0.47          |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD22 | 5        | 0.47          |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 15       | 0.47          |
| (2,1710) | 2:1789:A:ALA:HB2  | 2:1790:A:ALA:HA   | 17       | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 3        | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 4        | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 6        | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 7        | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 9        | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 10       | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 12       | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 15       | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 16       | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 17       | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 18       | 0.47          |
| (2,1647) | 2:1797:A:GLN:HG2  | 2:1797:A:GLN:HB2  | 19       | 0.47          |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 7        | 0.47          |
| (2,1526) | 2:1746:A:ALA:HB3  | 2:1804:A:PRO:HD2  | 9        | 0.47          |
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 2        | 0.47          |
| (2,1518) | 2:1764:A:VAL:HG11 | 2:1766:A:GLN:H    | 5        | 0.47          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 7        | 0.47          |
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 12       | 0.47          |
| (2,1518) | 2:1764:A:VAL:HG13 | 2:1766:A:GLN:H    | 19       | 0.47          |
| (2,1518) | 2:1764:A:VAL:HG12 | 2:1766:A:GLN:H    | 20       | 0.47          |
| (2,1501) | 2:1781:A:ILE:HD11 | 2:1780:A:PRO:HG2  | 19       | 0.47          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 13       | 0.47          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 14       | 0.47          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 13       | 0.47          |
| (2,1424) | 2:1778:A:GLY:HA2  | 2:1773:A:ARG:HB3  | 5        | 0.47          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG21 | 6        | 0.47          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 13       | 0.47          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 15       | 0.47          |
| (2,1346) | 2:1755:A:LEU:HD23 | 2:1758:A:CYS:HB3  | 3        | 0.47          |
| (2,1337) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HG2  | 18       | 0.47          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 1        | 0.47          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 4        | 0.47          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 8        | 0.47          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 12       | 0.47          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 6        | 0.47          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 6        | 0.47          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 9        | 0.47          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 18       | 0.47          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 19       | 0.47          |
| (2,1146) | 2:1788:A:LEU:HD23 | 2:1735:A:ILE:HA   | 16       | 0.47          |
| (2,1098) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HE2  | 5        | 0.47          |
| (2,1085) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:H    | 20       | 0.47          |
| (2,1084) | 2:1768:A:THR:HG21 | 2:1781:A:ILE:HG23 | 11       | 0.47          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG22  | 7        | 0.47          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 6        | 0.47          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG21 | 7        | 0.47          |
| (2,1005) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HG2  | 9        | 0.47          |
| (2,1002) | 2:1738:A:ALA:HB1  | 2:1739:A:ILE:HA   | 4        | 0.47          |
| (2,1002) | 2:1738:A:ALA:HB2  | 2:1739:A:ILE:HA   | 6        | 0.47          |
| (2,1002) | 2:1738:A:ALA:HB3  | 2:1739:A:ILE:HA   | 15       | 0.47          |
| (2,1002) | 2:1738:A:ALA:HB2  | 2:1739:A:ILE:HA   | 18       | 0.47          |
| (2,966)  | 2:1739:A:ILE:HD13 | 2:1788:A:LEU:HB2  | 8        | 0.47          |
| (2,966)  | 2:1739:A:ILE:HD11 | 2:1788:A:LEU:HB2  | 10       | 0.47          |
| (2,881)  | 2:1807:A:LEU:HG   | 2:1801:A:CYS:HB2  | 13       | 0.47          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 10       | 0.47          |
| (2,819)  | 2:1749:A:ARG:HA   | 2:1749:A:ARG:HD3  | 11       | 0.47          |
| (2,812)  | 2:1786:A:ILE:HG23 | 2:1783:A:LYS:HA   | 4        | 0.47          |
| (2,812)  | 2:1786:A:ILE:HG23 | 2:1783:A:LYS:HA   | 20       | 0.47          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 4        | 0.47          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 12       | 0.47          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 14       | 0.47          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 18       | 0.47          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 13       | 0.47          |
| (2,680)  | 1:138:B:MET:HG2   | 1:137:B:LEU:HD12  | 16       | 0.47          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 19       | 0.47          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG23  | 5        | 0.47          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 4        | 0.47          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 4        | 0.47          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG22  | 9        | 0.47          |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 8        | 0.47          |
| (2,249)  | 2:1781:A:ILE:HG22 | 2:1781:A:ILE:H    | 10       | 0.47          |
| (2,249)  | 2:1781:A:ILE:HG22 | 2:1781:A:ILE:H    | 18       | 0.47          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 4        | 0.47          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 8        | 0.47          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 16       | 0.47          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 19       | 0.47          |
| (2,99)   | 2:1745:A:ALA:HB3  | 2:1744:A:HIS:H    | 1        | 0.47          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 3        | 0.47          |
| (2,99)   | 2:1745:A:ALA:HB3  | 2:1744:A:HIS:H    | 10       | 0.47          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 1        | 0.47          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB3  | 12       | 0.47          |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 4        | 0.47          |
| (2,82)   | 2:1764:A:VAL:HG11 | 2:1764:A:VAL:H    | 14       | 0.47          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 7        | 0.47          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 15       | 0.47          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 16       | 0.47          |
| (2,1737) | 2:1785:A:LEU:HD13 | 2:1767:A:HIS:HD2  | 5        | 0.46          |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 4        | 0.46          |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 5        | 0.46          |
| (2,1710) | 2:1789:A:ALA:HB2  | 2:1790:A:ALA:HA   | 11       | 0.46          |
| (2,1699) | 2:1781:A:ILE:HD12 | 2:1767:A:HIS:HD2  | 4        | 0.46          |
| (2,1699) | 2:1781:A:ILE:HD13 | 2:1767:A:HIS:HD2  | 19       | 0.46          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 9        | 0.46          |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 6        | 0.46          |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 1        | 0.46          |
| (2,1607) | 2:1781:A:ILE:HD11 | 2:1782:A:CYS:H    | 9        | 0.46          |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 14       | 0.46          |
| (2,1518) | 2:1764:A:VAL:HG11 | 2:1766:A:GLN:H    | 14       | 0.46          |
| (2,1518) | 2:1764:A:VAL:HG11 | 2:1766:A:GLN:H    | 18       | 0.46          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 1        | 0.46          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 2        | 0.46          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 10       | 0.46          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 12       | 0.46          |
| (2,1415) | 2:1735:A:ILE:HD12 | 2:1735:A:ILE:H    | 7        | 0.46          |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 18       | 0.46          |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 19       | 0.46          |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG23 | 8        | 0.46          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 2        | 0.46          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 12       | 0.46          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 14       | 0.46          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 17       | 0.46          |
| (2,1228) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:HA   | 17       | 0.46          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 5        | 0.46          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 14       | 0.46          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 15       | 0.46          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 9        | 0.46          |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 11       | 0.46          |
| (2,1098) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HE2  | 6        | 0.46          |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 13       | 0.46          |
| (2,1085) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:H    | 19       | 0.46          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG22  | 9        | 0.46          |
| (2,1002) | 2:1738:A:ALA:HB2  | 2:1739:A:ILE:HA   | 8        | 0.46          |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG23 | 2        | 0.46          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 8        | 0.46          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 14       | 0.46          |
| (2,966)  | 2:1739:A:ILE:HD12 | 2:1788:A:LEU:HB2  | 17       | 0.46          |
| (2,966)  | 2:1739:A:ILE:HD13 | 2:1788:A:LEU:HB2  | 18       | 0.46          |
| (2,919)  | 2:1765:A:VAL:HG21 | 2:1762:A:LYS:HA   | 15       | 0.46          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD12 | 2        | 0.46          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 19       | 0.46          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 14       | 0.46          |
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 1        | 0.46          |
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 7        | 0.46          |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 8        | 0.46          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 2        | 0.46          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 19       | 0.46          |
| (2,733)  | 2:1734:A:SER:HB3  | 2:1734:A:SER:H    | 20       | 0.46          |
| (2,726)  | 2:1746:A:ALA:HB1  | 2:1765:A:VAL:HG12 | 12       | 0.46          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 10       | 0.46          |
| (2,679)  | 1:135:B:LEU:HD12  | 1:132:B:GLU:HA    | 19       | 0.46          |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE2   | 4        | 0.46          |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE2   | 13       | 0.46          |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG21  | 2        | 0.46          |
| (2,558)  | 1:120:B:ILE:HD12  | 1:120:B:ILE:H     | 10       | 0.46          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 17       | 0.46          |
| (2,558)  | 1:120:B:ILE:HD12  | 1:120:B:ILE:H     | 20       | 0.46          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 16       | 0.46          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 5        | 0.46          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 8        | 0.46          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD12  | 20       | 0.46          |
| (2,268)  | 2:1773:A:ARG:H    | 2:1773:A:ARG:HD3  | 18       | 0.46          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 4        | 0.46          |
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 5        | 0.46          |
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 15       | 0.46          |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 17       | 0.46          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 10       | 0.46          |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 8        | 0.46          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 15       | 0.46          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 1        | 0.46          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 2        | 0.46          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 5        | 0.46          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 7        | 0.46          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 18       | 0.46          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 20       | 0.46          |
| (2,120)  | 2:1752:A:ASN:H    | 2:1752:A:ASN:HD22 | 19       | 0.46          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 9        | 0.46          |
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 17       | 0.46          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 10       | 0.46          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD2  | 17       | 0.45          |
| (2,1698) | 2:1788:A:LEU:HD23 | 2:1787:A:ALA:H    | 19       | 0.45          |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 2        | 0.45          |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE2  | 19       | 0.45          |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 4        | 0.45          |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 8        | 0.45          |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 13       | 0.45          |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 2        | 0.45          |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 19       | 0.45          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD13 | 19       | 0.45          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG22 | 14       | 0.45          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 3        | 0.45          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 5        | 0.45          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG21 | 6        | 0.45          |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD1  | 20       | 0.45          |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 2        | 0.45          |
| (2,1415) | 2:1735:A:ILE:HD12 | 2:1735:A:ILE:H    | 16       | 0.45          |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG22 | 5        | 0.45          |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG13 | 17       | 0.45          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 11       | 0.45          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 15       | 0.45          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 17       | 0.45          |
| (2,1255) | 2:1725:A:GLN:HA   | 2:1725:A:GLN:HG2  | 5        | 0.45          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 8        | 0.45          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 10       | 0.45          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 16       | 0.45          |
| (2,1244) | 2:1775:A:THR:HG23 | 2:1776:A:ASN:HB2  | 8        | 0.45          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 1        | 0.45          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 10       | 0.45          |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 12       | 0.45          |
| (2,1130) | 2:1761:A:MET:HE3  | 2:1739:A:ILE:HA   | 7        | 0.45          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 20       | 0.45          |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG21 | 7        | 0.45          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 10       | 0.45          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 17       | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 2        | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 3        | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 4        | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 5        | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 6        | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 7        | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 8        | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 11       | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 12       | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 14       | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 15       | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 16       | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 19       | 0.45          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 20       | 0.45          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD11 | 1        | 0.45          |
| (2,881)  | 2:1807:A:LEU:HG   | 2:1801:A:CYS:HB2  | 20       | 0.45          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 12       | 0.45          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 3        | 0.45          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 9        | 0.45          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 11       | 0.45          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 20       | 0.45          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD22 | 9        | 0.45          |
| (2,669)  | 1:120:B:ILE:HG21  | 1:117:B:ASP:H     | 14       | 0.45          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 7        | 0.45          |
| (2,538)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HB2   | 18       | 0.45          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 13       | 0.45          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 3        | 0.45          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 18       | 0.45          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG21  | 15       | 0.45          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 18       | 0.45          |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 1        | 0.45          |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 3        | 0.45          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 9        | 0.45          |
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 11       | 0.45          |
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 16       | 0.45          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 6        | 0.45          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 12       | 0.45          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 10       | 0.45          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 14       | 0.45          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 8        | 0.45          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB2  | 6        | 0.45          |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 6        | 0.45          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 8        | 0.45          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 1        | 0.45          |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 10       | 0.44          |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 12       | 0.44          |
| (2,1710) | 2:1789:A:ALA:HB2  | 2:1790:A:ALA:HA   | 16       | 0.44          |
| (2,1698) | 2:1788:A:LEU:HD21 | 2:1787:A:ALA:H    | 4        | 0.44          |
| (2,1639) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:H    | 3        | 0.44          |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 6        | 0.44          |
| (2,1551) | 2:1735:A:ILE:HG23 | 2:1791:A:TYR:HB2  | 18       | 0.44          |
| (2,1526) | 2:1746:A:ALA:HB3  | 2:1804:A:PRO:HD2  | 18       | 0.44          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 7        | 0.44          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 17       | 0.44          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 1        | 0.44          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 8        | 0.44          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 15       | 0.44          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 7        | 0.44          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 7        | 0.44          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB1  | 20       | 0.44          |
| (2,1415) | 2:1735:A:ILE:HD12 | 2:1735:A:ILE:H    | 14       | 0.44          |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG22 | 12       | 0.44          |
| (2,1385) | 2:1785:A:LEU:HD12 | 2:1768:A:THR:HG21 | 15       | 0.44          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 5        | 0.44          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG11 | 9        | 0.44          |
| (2,1130) | 2:1761:A:MET:HE3  | 2:1739:A:ILE:HA   | 15       | 0.44          |
| (2,1001) | 2:1738:A:ALA:HB1  | 2:1735:A:ILE:HG23 | 16       | 0.44          |
| (2,1001) | 2:1738:A:ALA:HB3  | 2:1735:A:ILE:HG22 | 19       | 0.44          |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 9        | 0.44          |
| (2,966)  | 2:1739:A:ILE:HD11 | 2:1788:A:LEU:HB2  | 13       | 0.44          |
| (2,947)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:HG2  | 13       | 0.44          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 13       | 0.44          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 15       | 0.44          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 16       | 0.44          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 6        | 0.44          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 7        | 0.44          |
| (2,726)  | 2:1746:A:ALA:HB2  | 2:1765:A:VAL:HG12 | 8        | 0.44          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 18       | 0.44          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 13       | 0.44          |
| (2,685)  | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG2  | 17       | 0.44          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 9        | 0.44          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 17       | 0.44          |
| (2,540)  | 1:134:B:ILE:HG21  | 2:1781:A:ILE:HA   | 1        | 0.44          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG23  | 5        | 0.44          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 20       | 0.44          |
| (2,249)  | 2:1781:A:ILE:HG21 | 2:1781:A:ILE:H    | 12       | 0.44          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 8        | 0.44          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 14       | 0.44          |
| (2,154)  | 2:1759:A:GLN:H    | 2:1759:A:GLN:HB2  | 9        | 0.44          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 12       | 0.44          |
| (2,99)   | 2:1745:A:ALA:HB3  | 2:1744:A:HIS:H    | 12       | 0.44          |
| (2,99)   | 2:1745:A:ALA:HB1  | 2:1744:A:HIS:H    | 20       | 0.44          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB3  | 3        | 0.44          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 2        | 0.44          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 3        | 0.44          |
| (3,12)   | 1:123:B:ILE:HA    | 1:126:B:LEU:HD21  | 16       | 0.43          |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD23 | 17       | 0.43          |
| (2,1737) | 2:1785:A:LEU:HD12 | 2:1767:A:HIS:HD2  | 18       | 0.43          |
| (2,1710) | 2:1789:A:ALA:HB2  | 2:1790:A:ALA:HA   | 18       | 0.43          |
| (2,1699) | 2:1781:A:ILE:HD11 | 2:1767:A:HIS:HD2  | 18       | 0.43          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 8        | 0.43          |
| (2,1655) | 2:1787:A:ALA:HB2  | 2:1784:A:GLN:HB3  | 17       | 0.43          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 13       | 0.43          |
| (2,1607) | 2:1781:A:ILE:HD11 | 2:1782:A:CYS:H    | 5        | 0.43          |
| (2,1607) | 2:1781:A:ILE:HD11 | 2:1782:A:CYS:H    | 19       | 0.43          |
| (2,1607) | 2:1781:A:ILE:HD11 | 2:1782:A:CYS:H    | 20       | 0.43          |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 13       | 0.43          |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 17       | 0.43          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 9        | 0.43          |
| (2,1478) | 2:1789:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 15       | 0.43          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG23 | 4        | 0.43          |
| (2,1464) | 2:1742:A:LEU:HG   | 2:1803:A:VAL:HG21 | 16       | 0.43          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 17       | 0.43          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 5        | 0.43          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB3  | 4        | 0.43          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 5        | 0.43          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 12       | 0.43          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB3  | 13       | 0.43          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 19       | 0.43          |
| (2,1346) | 2:1755:A:LEU:HD21 | 2:1758:A:CYS:HB3  | 9        | 0.43          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 9        | 0.43          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 13       | 0.43          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 2        | 0.43          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 16       | 0.43          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 17       | 0.43          |
| (2,1207) | 2:1763:A:ARG:HB3  | 2:1760:A:LYS:HA   | 2        | 0.43          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 9        | 0.43          |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 4        | 0.43          |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 17       | 0.43          |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 18       | 0.43          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 9        | 0.43          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 8        | 0.43          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 6        | 0.43          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 2        | 0.43          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 3        | 0.43          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 1        | 0.43          |
| (2,919)  | 2:1765:A:VAL:HG22 | 2:1762:A:LYS:HA   | 3        | 0.43          |
| (2,919)  | 2:1765:A:VAL:HG22 | 2:1762:A:LYS:HA   | 12       | 0.43          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 8        | 0.43          |
| (2,819)  | 2:1749:A:ARG:HA   | 2:1749:A:ARG:HD3  | 1        | 0.43          |
| (2,726)  | 2:1746:A:ALA:HB1  | 2:1765:A:VAL:HG13 | 6        | 0.43          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 11       | 0.43          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 16       | 0.43          |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG21  | 19       | 0.43          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 3        | 0.43          |
| (2,465)  | 1:137:B:LEU:HD23  | 1:138:B:MET:H     | 19       | 0.43          |
| (2,463)  | 1:134:B:ILE:HD11  | 1:134:B:ILE:H     | 17       | 0.43          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 3        | 0.43          |
| (2,249)  | 2:1781:A:ILE:HG23 | 2:1781:A:ILE:H    | 2        | 0.43          |
| (2,192)  | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG21  | 18       | 0.43          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 13       | 0.43          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 15       | 0.43          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 8        | 0.43          |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 15       | 0.43          |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 20       | 0.43          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 13       | 0.43          |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD23 | 6        | 0.42          |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD23 | 9        | 0.42          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1699) | 2:1781:A:ILE:HD13 | 2:1767:A:HIS:HD2  | 5        | 0.42          |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 3        | 0.42          |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 17       | 0.42          |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 4        | 0.42          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 19       | 0.42          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 1        | 0.42          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB3  | 6        | 0.42          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 8        | 0.42          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB1  | 10       | 0.42          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB1  | 11       | 0.42          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB1  | 14       | 0.42          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 16       | 0.42          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB3  | 17       | 0.42          |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 4        | 0.42          |
| (2,1407) | 2:1804:A:PRO:HG2  | 2:1803:A:VAL:HG22 | 19       | 0.42          |
| (2,1396) | 2:1793:A:ALA:HB3  | 2:1796:A:CYS:HB3  | 13       | 0.42          |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG12 | 10       | 0.42          |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG11 | 16       | 0.42          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 2        | 0.42          |
| (2,1308) | 2:1811:A:GLN:HB2  | 2:1811:A:GLN:HG3  | 4        | 0.42          |
| (2,1308) | 2:1811:A:GLN:HB2  | 2:1811:A:GLN:HG3  | 13       | 0.42          |
| (2,1308) | 2:1811:A:GLN:HB2  | 2:1811:A:GLN:HG3  | 17       | 0.42          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 3        | 0.42          |
| (2,1244) | 2:1775:A:THR:HG23 | 2:1776:A:ASN:HB2  | 2        | 0.42          |
| (2,1213) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:H    | 8        | 0.42          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 11       | 0.42          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 7        | 0.42          |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 4        | 0.42          |
| (2,1081) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HG   | 18       | 0.42          |
| (2,1052) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HE2  | 17       | 0.42          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 2        | 0.42          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 8        | 0.42          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 16       | 0.42          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 4        | 0.42          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 14       | 0.42          |
| (2,936)  | 2:1732:A:ARG:HG2  | 2:1732:A:ARG:HA   | 15       | 0.42          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 8        | 0.42          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 6        | 0.42          |
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 3        | 0.42          |
| (2,812)  | 2:1786:A:ILE:HG23 | 2:1783:A:LYS:HA   | 19       | 0.42          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 9        | 0.42          |
| (2,763)  | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 12       | 0.42          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1   | 7        | 0.42          |
| (2,538)  | 1:126:B:LEU:HD11  | 1:126:B:LEU:HB2   | 1        | 0.42          |
| (2,538)  | 1:126:B:LEU:HD12  | 1:126:B:LEU:HB2   | 3        | 0.42          |
| (2,538)  | 1:126:B:LEU:HD13  | 1:126:B:LEU:HB2   | 16       | 0.42          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 4        | 0.42          |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG21  | 10       | 0.42          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 7        | 0.42          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 10       | 0.42          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 10       | 0.42          |
| (2,374)  | 1:127:B:GLU:H     | 1:126:B:LEU:HD11  | 6        | 0.42          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB3  | 1        | 0.42          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB2  | 9        | 0.42          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 13       | 0.42          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 11       | 0.42          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 17       | 0.42          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 9        | 0.42          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 13       | 0.42          |
| (3,8)    | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD21 | 15       | 0.41          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 11       | 0.41          |
| (2,1710) | 2:1789:A:ALA:HB3  | 2:1790:A:ALA:HA   | 7        | 0.41          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 12       | 0.41          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 7        | 0.41          |
| (2,1655) | 2:1787:A:ALA:HB3  | 2:1784:A:GLN:HB3  | 11       | 0.41          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 12       | 0.41          |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 7        | 0.41          |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 10       | 0.41          |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 15       | 0.41          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 3        | 0.41          |
| (2,1529) | 2:1746:A:ALA:HB3  | 2:1747:A:GLN:HG3  | 19       | 0.41          |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 16       | 0.41          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 4        | 0.41          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 12       | 0.41          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 16       | 0.41          |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 18       | 0.41          |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 12       | 0.41          |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 17       | 0.41          |
| (2,1394) | 2:1793:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 11       | 0.41          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 5        | 0.41          |
| (2,1265) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HG3  | 18       | 0.41          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 20       | 0.41          |
| (2,1244) | 2:1775:A:THR:HG21 | 2:1776:A:ASN:HB2  | 20       | 0.41          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 18       | 0.41          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD2   | 14       | 0.41          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 10       | 0.41          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 14       | 0.41          |
| (2,1130) | 2:1761:A:MET:HE3  | 2:1739:A:ILE:HA   | 18       | 0.41          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 8        | 0.41          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 14       | 0.41          |
| (2,1081) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HG   | 15       | 0.41          |
| (2,1001) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HG23 | 14       | 0.41          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 6        | 0.41          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 13       | 0.41          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 11       | 0.41          |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG22 | 11       | 0.41          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 12       | 0.41          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 18       | 0.41          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 2        | 0.41          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 1        | 0.41          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 5        | 0.41          |
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 2        | 0.41          |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 5        | 0.41          |
| (2,812)  | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 11       | 0.41          |
| (2,669)  | 1:120:B:ILE:HG22  | 1:117:B:ASP:H     | 2        | 0.41          |
| (2,648)  | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG21  | 19       | 0.41          |
| (2,646)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HD1   | 7        | 0.41          |
| (2,617)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:HA    | 3        | 0.41          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 4        | 0.41          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 13       | 0.41          |
| (2,559)  | 1:134:B:ILE:HD11  | 1:131:B:ASN:HD21  | 15       | 0.41          |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD21  | 20       | 0.41          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 11       | 0.41          |
| (2,387)  | 1:116:B:MET:H     | 1:115:B:GLN:HB2   | 18       | 0.41          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG21  | 6        | 0.41          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG23  | 10       | 0.41          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG22  | 18       | 0.41          |
| (2,275)  | 2:1778:A:GLY:H    | 2:1776:A:ASN:HB2  | 14       | 0.41          |
| (2,275)  | 2:1778:A:GLY:H    | 2:1776:A:ASN:HB2  | 15       | 0.41          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 13       | 0.41          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 15       | 0.41          |
| (2,192)  | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG21  | 19       | 0.41          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 10       | 0.41          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 14       | 0.41          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 19       | 0.41          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 20       | 0.41          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 5        | 0.41          |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 7        | 0.41          |
| (2,82)   | 2:1764:A:VAL:HG12 | 2:1764:A:VAL:H    | 13       | 0.41          |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD23 | 8        | 0.4           |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 1        | 0.4           |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 16       | 0.4           |
| (2,1607) | 2:1781:A:ILE:HD11 | 2:1782:A:CYS:H    | 1        | 0.4           |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 3        | 0.4           |
| (2,1555) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HD1   | 8        | 0.4           |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 10       | 0.4           |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 14       | 0.4           |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 11       | 0.4           |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 20       | 0.4           |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD11 | 3        | 0.4           |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 9        | 0.4           |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD11 | 19       | 0.4           |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 1        | 0.4           |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 2        | 0.4           |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 3        | 0.4           |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB3  | 9        | 0.4           |
| (2,1429) | 2:1787:A:ALA:HA   | 2:1787:A:ALA:HB2  | 15       | 0.4           |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 8        | 0.4           |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 15       | 0.4           |
| (2,1387) | 2:1785:A:LEU:HD13 | 2:1805:A:PHE:HE2  | 5        | 0.4           |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 19       | 0.4           |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 6        | 0.4           |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 9        | 0.4           |
| (2,1150) | 2:1743:A:VAL:HG21 | 2:1803:A:VAL:HG12 | 7        | 0.4           |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 12       | 0.4           |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 5        | 0.4           |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 14       | 0.4           |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 17       | 0.4           |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG23 | 2        | 0.4           |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 1        | 0.4           |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 4        | 0.4           |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 10       | 0.4           |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 12       | 0.4           |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 14       | 0.4           |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 17       | 0.4           |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 20       | 0.4           |
| (2,987)  | 2:1764:A:VAL:HA   | 2:1781:A:ILE:HG23 | 19       | 0.4           |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 5        | 0.4           |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (2,968) | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 16       | 0.4           |
| (2,968) | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 17       | 0.4           |
| (2,963) | 2:1739:A:ILE:HD12 | 2:1792:A:HIS:HB3  | 9        | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 3        | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 6        | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 7        | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 8        | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 9        | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 10       | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 13       | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 14       | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 15       | 0.4           |
| (2,935) | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 20       | 0.4           |
| (2,929) | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 1        | 0.4           |
| (2,929) | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD22 | 5        | 0.4           |
| (2,919) | 2:1765:A:VAL:HG22 | 2:1762:A:LYS:HA   | 11       | 0.4           |
| (2,894) | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD11 | 16       | 0.4           |
| (2,862) | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD12 | 1        | 0.4           |
| (2,862) | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD12 | 16       | 0.4           |
| (2,857) | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 18       | 0.4           |
| (2,812) | 2:1786:A:ILE:HG22 | 2:1783:A:LYS:HA   | 12       | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 3        | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 4        | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 5        | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 6        | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 8        | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 9        | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 13       | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 14       | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 15       | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 18       | 0.4           |
| (2,634) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 19       | 0.4           |
| (2,517) | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD22  | 2        | 0.4           |
| (2,517) | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD21  | 6        | 0.4           |
| (2,431) | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 1        | 0.4           |
| (2,431) | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 3        | 0.4           |
| (2,359) | 1:121:B:ASP:H     | 1:120:B:ILE:HG22  | 2        | 0.4           |
| (2,359) | 1:121:B:ASP:H     | 1:120:B:ILE:HG23  | 4        | 0.4           |
| (2,215) | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 18       | 0.4           |
| (2,105) | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 5        | 0.4           |
| (2,105) | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 6        | 0.4           |
| (2,105) | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 17       | 0.4           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 19       | 0.4           |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 5        | 0.39          |
| (2,1699) | 2:1781:A:ILE:HD12 | 2:1767:A:HIS:HD2  | 15       | 0.39          |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 8        | 0.39          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 19       | 0.39          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 10       | 0.39          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 3        | 0.39          |
| (2,1526) | 2:1746:A:ALA:HB1  | 2:1804:A:PRO:HD2  | 11       | 0.39          |
| (2,1526) | 2:1746:A:ALA:HB2  | 2:1804:A:PRO:HD2  | 20       | 0.39          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 6        | 0.39          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 18       | 0.39          |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG12 | 2        | 0.39          |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG11 | 9        | 0.39          |
| (2,1346) | 2:1755:A:LEU:HD21 | 2:1758:A:CYS:HB3  | 5        | 0.39          |
| (2,1244) | 2:1775:A:THR:HG22 | 2:1776:A:ASN:HB2  | 1        | 0.39          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG12 | 8        | 0.39          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 2        | 0.39          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 15       | 0.39          |
| (2,1083) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HD22 | 19       | 0.39          |
| (2,1081) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HG   | 1        | 0.39          |
| (2,1081) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HG   | 12       | 0.39          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 9        | 0.39          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 15       | 0.39          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 18       | 0.39          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 19       | 0.39          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 5        | 0.39          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD13 | 11       | 0.39          |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 2        | 0.39          |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 8        | 0.39          |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 10       | 0.39          |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 15       | 0.39          |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 19       | 0.39          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 1        | 0.39          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 4        | 0.39          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 5        | 0.39          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 11       | 0.39          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 16       | 0.39          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 19       | 0.39          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 7        | 0.39          |
| (2,899)  | 2:1768:A:THR:HA   | 2:1771:A:CYS:HB2  | 11       | 0.39          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 16       | 0.39          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 17       | 0.39          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,850)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB3  | 18       | 0.39          |
| (2,812)  | 2:1786:A:ILE:HG23 | 2:1783:A:LYS:HA   | 15       | 0.39          |
| (2,812)  | 2:1786:A:ILE:HG23 | 2:1783:A:LYS:HA   | 16       | 0.39          |
| (2,812)  | 2:1786:A:ILE:HG21 | 2:1783:A:LYS:HA   | 18       | 0.39          |
| (2,666)  | 1:120:B:ILE:HD13  | 1:117:B:ASP:HB3   | 12       | 0.39          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 9        | 0.39          |
| (2,634)  | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 2        | 0.39          |
| (2,634)  | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 10       | 0.39          |
| (2,634)  | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 16       | 0.39          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 8        | 0.39          |
| (2,559)  | 1:134:B:ILE:HD11  | 1:131:B:ASN:HD21  | 5        | 0.39          |
| (2,559)  | 1:134:B:ILE:HD13  | 1:131:B:ASN:HD21  | 18       | 0.39          |
| (2,558)  | 1:120:B:ILE:HD12  | 1:120:B:ILE:H     | 3        | 0.39          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 17       | 0.39          |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD21  | 9        | 0.39          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 12       | 0.39          |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 12       | 0.39          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 2        | 0.39          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 7        | 0.39          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 19       | 0.39          |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 18       | 0.39          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG23  | 17       | 0.39          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB3  | 2        | 0.39          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 11       | 0.39          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 20       | 0.39          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 19       | 0.39          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 6        | 0.39          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 4        | 0.39          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 15       | 0.39          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 15       | 0.39          |
| (2,82)   | 2:1764:A:VAL:HG13 | 2:1764:A:VAL:H    | 10       | 0.39          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 14       | 0.38          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 3        | 0.38          |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD23 | 4        | 0.38          |
| (2,1677) | 2:1767:A:HIS:HB3  | 2:1781:A:ILE:HG23 | 19       | 0.38          |
| (2,1655) | 2:1787:A:ALA:HB3  | 2:1784:A:GLN:HB3  | 10       | 0.38          |
| (2,1655) | 2:1787:A:ALA:HB3  | 2:1784:A:GLN:HB3  | 20       | 0.38          |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 2        | 0.38          |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 16       | 0.38          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 17       | 0.38          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 15       | 0.38          |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 13       | 0.38          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1514) | 2:1764:A:VAL:HG13 | 2:1781:A:ILE:HG22 | 18       | 0.38          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG21 | 4        | 0.38          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 7        | 0.38          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 10       | 0.38          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 8        | 0.38          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 10       | 0.38          |
| (2,1346) | 2:1755:A:LEU:HD23 | 2:1758:A:CYS:HB3  | 15       | 0.38          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB1  | 7        | 0.38          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 15       | 0.38          |
| (2,1228) | 2:1812:A:LYS:HD3  | 2:1812:A:LYS:HA   | 10       | 0.38          |
| (2,1153) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HG2  | 1        | 0.38          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG11 | 4        | 0.38          |
| (2,1148) | 2:1788:A:LEU:HD21 | 1:130:B:TYR:HD2   | 11       | 0.38          |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD2   | 18       | 0.38          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 2        | 0.38          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 4        | 0.38          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 17       | 0.38          |
| (2,1069) | 2:1768:A:THR:HG21 | 2:1785:A:LEU:HD23 | 10       | 0.38          |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 4        | 0.38          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 19       | 0.38          |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 8        | 0.38          |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 14       | 0.38          |
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 15       | 0.38          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 3        | 0.38          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 5        | 0.38          |
| (2,968)  | 2:1800:A:LYS:HD3  | 2:1800:A:LYS:HE2  | 20       | 0.38          |
| (2,951)  | 2:1780:A:PRO:HB3  | 1:134:B:ILE:HG22  | 12       | 0.38          |
| (2,936)  | 2:1732:A:ARG:HG2  | 2:1732:A:ARG:HA   | 13       | 0.38          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 2        | 0.38          |
| (2,935)  | 2:1732:A:ARG:HA   | 2:1732:A:ARG:HB3  | 17       | 0.38          |
| (2,919)  | 2:1765:A:VAL:HG22 | 2:1762:A:LYS:HA   | 9        | 0.38          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 18       | 0.38          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 20       | 0.38          |
| (2,881)  | 2:1807:A:LEU:HG   | 2:1801:A:CYS:HB2  | 17       | 0.38          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 6        | 0.38          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 2        | 0.38          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 15       | 0.38          |
| (2,838)  | 2:1745:A:ALA:HA   | 2:1762:A:LYS:HE2  | 11       | 0.38          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 12       | 0.38          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 3        | 0.38          |
| (2,634)  | 1:115:B:GLN:HG2   | 1:115:B:GLN:HB2   | 7        | 0.38          |
| (2,617)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:HA    | 13       | 0.38          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 3        | 0.38          |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG22  | 9        | 0.38          |
| (2,559)  | 1:134:B:ILE:HD12  | 1:131:B:ASN:HD21  | 7        | 0.38          |
| (2,558)  | 1:120:B:ILE:HD12  | 1:120:B:ILE:H     | 12       | 0.38          |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD23  | 8        | 0.38          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 20       | 0.38          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 8        | 0.38          |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 7        | 0.38          |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 15       | 0.38          |
| (2,238)  | 2:1779:A:CYS:H    | 2:1773:A:ARG:HD3  | 9        | 0.38          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 9        | 0.38          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 10       | 0.38          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 7        | 0.38          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 12       | 0.37          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 13       | 0.37          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 9        | 0.37          |
| (2,1727) | 2:1781:A:ILE:HG21 | 2:1767:A:HIS:HD2  | 15       | 0.37          |
| (2,1710) | 2:1789:A:ALA:HB1  | 2:1790:A:ALA:HA   | 2        | 0.37          |
| (2,1699) | 2:1781:A:ILE:HD13 | 2:1767:A:HIS:HD2  | 9        | 0.37          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 16       | 0.37          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 1        | 0.37          |
| (2,1655) | 2:1787:A:ALA:HB2  | 2:1784:A:GLN:HB3  | 4        | 0.37          |
| (2,1655) | 2:1787:A:ALA:HB2  | 2:1784:A:GLN:HB3  | 13       | 0.37          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 4        | 0.37          |
| (2,1529) | 2:1746:A:ALA:HB2  | 2:1747:A:GLN:HG3  | 12       | 0.37          |
| (2,1529) | 2:1746:A:ALA:HB2  | 2:1747:A:GLN:HG3  | 18       | 0.37          |
| (2,1515) | 2:1764:A:VAL:HG12 | 2:1761:A:MET:HG2  | 14       | 0.37          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 2        | 0.37          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 13       | 0.37          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 17       | 0.37          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 6        | 0.37          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD11 | 11       | 0.37          |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG11 | 4        | 0.37          |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG12 | 15       | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 2        | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 4        | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 5        | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 11       | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 13       | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 14       | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 15       | 0.37          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 17       | 0.37          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 15       | 0.37          |
| (2,1146) | 2:1788:A:LEU:HD23 | 2:1735:A:ILE:HA   | 8        | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 5        | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 6        | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 7        | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 8        | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 9        | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 10       | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 11       | 0.37          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 14       | 0.37          |
| (2,1085) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:H    | 18       | 0.37          |
| (2,1083) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HD23 | 20       | 0.37          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 1        | 0.37          |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 6        | 0.37          |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 7        | 0.37          |
| (2,997)  | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:H    | 11       | 0.37          |
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 17       | 0.37          |
| (2,994)  | 2:1794:A:LYS:HA   | 2:1794:A:LYS:HG3  | 7        | 0.37          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 15       | 0.37          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 7        | 0.37          |
| (2,919)  | 2:1765:A:VAL:HG21 | 2:1762:A:LYS:HA   | 13       | 0.37          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 16       | 0.37          |
| (2,919)  | 2:1765:A:VAL:HG22 | 2:1762:A:LYS:HA   | 19       | 0.37          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 8        | 0.37          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 15       | 0.37          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG21 | 19       | 0.37          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 5        | 0.37          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 10       | 0.37          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 19       | 0.37          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 9        | 0.37          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 16       | 0.37          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 13       | 0.37          |
| (2,387)  | 1:116:B:MET:H     | 1:115:B:GLN:HB2   | 14       | 0.37          |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 10       | 0.37          |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 11       | 0.37          |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 16       | 0.37          |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 1        | 0.37          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 2        | 0.37          |
| (2,215)  | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 16       | 0.37          |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 1        | 0.37          |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 3        | 0.37          |
| (2,133)  | 2:1733:A:LEU:HB3  | 2:1734:A:SER:H    | 9        | 0.37          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 6        | 0.37          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 17       | 0.37          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 1        | 0.37          |
| (2,1655) | 2:1787:A:ALA:HB2  | 2:1784:A:GLN:HB3  | 6        | 0.36          |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 19       | 0.36          |
| (2,1607) | 2:1781:A:ILE:HD11 | 2:1782:A:CYS:H    | 12       | 0.36          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 13       | 0.36          |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 15       | 0.36          |
| (2,1478) | 2:1789:A:ALA:HB3  | 2:1809:A:ILE:HD12 | 4        | 0.36          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG21 | 9        | 0.36          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG22 | 16       | 0.36          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD11 | 18       | 0.36          |
| (2,1379) | 2:1809:A:ILE:HG23 | 2:1793:A:ALA:HB2  | 18       | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 1        | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 3        | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 6        | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 7        | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 8        | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 9        | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 10       | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 12       | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 16       | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 18       | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 19       | 0.36          |
| (2,1350) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:HB3  | 20       | 0.36          |
| (2,1244) | 2:1775:A:THR:HG21 | 2:1776:A:ASN:HB2  | 3        | 0.36          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 4        | 0.36          |
| (2,1153) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HG2  | 7        | 0.36          |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 15       | 0.36          |
| (2,1136) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:H    | 9        | 0.36          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 19       | 0.36          |
| (2,1130) | 2:1761:A:MET:HE3  | 2:1739:A:ILE:HA   | 20       | 0.36          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 20       | 0.36          |
| (2,1089) | 2:1774:A:LYS:HA   | 2:1779:A:CYS:HB2  | 15       | 0.36          |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 12       | 0.36          |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 15       | 0.36          |
| (2,1081) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HG   | 2        | 0.36          |
| (2,1081) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HG   | 5        | 0.36          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 8        | 0.36          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG22 | 13       | 0.36          |
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 10       | 0.36          |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 12       | 0.36          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (2,997) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:H    | 18       | 0.36          |
| (2,997) | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:H    | 20       | 0.36          |
| (2,986) | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG13 | 18       | 0.36          |
| (2,971) | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 1        | 0.36          |
| (2,960) | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG21 | 5        | 0.36          |
| (2,937) | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD12 | 7        | 0.36          |
| (2,919) | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 10       | 0.36          |
| (2,882) | 2:1807:A:LEU:HG   | 2:1807:A:LEU:H    | 8        | 0.36          |
| (2,874) | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG21 | 1        | 0.36          |
| (2,874) | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG21 | 9        | 0.36          |
| (2,874) | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 13       | 0.36          |
| (2,862) | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 9        | 0.36          |
| (2,857) | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 7        | 0.36          |
| (2,850) | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB3  | 5        | 0.36          |
| (2,838) | 2:1745:A:ALA:HA   | 2:1762:A:LYS:HE2  | 20       | 0.36          |
| (2,750) | 2:1812:A:LYS:HG2  | 2:1812:A:LYS:H    | 1        | 0.36          |
| (2,722) | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD22 | 5        | 0.36          |
| (2,722) | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 7        | 0.36          |
| (2,685) | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG2  | 1        | 0.36          |
| (2,685) | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG2  | 12       | 0.36          |
| (2,672) | 1:129:B:SER:HA    | 1:132:B:GLU:HG2   | 8        | 0.36          |
| (2,669) | 1:120:B:ILE:HG23  | 1:117:B:ASP:H     | 4        | 0.36          |
| (2,652) | 1:127:B:GLU:HA    | 1:130:B:TYR:HD2   | 4        | 0.36          |
| (2,652) | 1:127:B:GLU:HA    | 1:130:B:TYR:HD2   | 13       | 0.36          |
| (2,648) | 1:131:B:ASN:HB2   | 1:134:B:ILE:HG22  | 18       | 0.36          |
| (2,617) | 1:137:B:LEU:HD21  | 1:137:B:LEU:HA    | 19       | 0.36          |
| (2,475) | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 1        | 0.36          |
| (2,397) | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 4        | 0.36          |
| (2,394) | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 7        | 0.36          |
| (2,394) | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 15       | 0.36          |
| (2,380) | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 1        | 0.36          |
| (2,380) | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 8        | 0.36          |
| (2,380) | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 20       | 0.36          |
| (2,273) | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 17       | 0.36          |
| (2,247) | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 8        | 0.36          |
| (2,215) | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 5        | 0.36          |
| (2,215) | 2:1755:A:LEU:H    | 2:1753:A:CYS:HB2  | 7        | 0.36          |
| (2,196) | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 6        | 0.36          |
| (2,105) | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 3        | 0.36          |
| (2,105) | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 16       | 0.36          |
| (2,82)  | 2:1764:A:VAL:HG11 | 2:1764:A:VAL:H    | 18       | 0.36          |
| (3,8)   | 2:1808:A:ASN:H    | 2:1807:A:LEU:HD21 | 5        | 0.35          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 4        | 0.35          |
| (2,1737) | 2:1785:A:LEU:HD12 | 2:1767:A:HIS:HD2  | 15       | 0.35          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 2        | 0.35          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 20       | 0.35          |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG23 | 18       | 0.35          |
| (2,1655) | 2:1787:A:ALA:HB3  | 2:1784:A:GLN:HB3  | 14       | 0.35          |
| (2,1555) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HD1   | 10       | 0.35          |
| (2,1551) | 2:1735:A:ILE:HG22 | 2:1791:A:TYR:HB2  | 2        | 0.35          |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 12       | 0.35          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 14       | 0.35          |
| (2,1415) | 2:1735:A:ILE:HD12 | 2:1735:A:ILE:H    | 20       | 0.35          |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG13 | 5        | 0.35          |
| (2,1346) | 2:1755:A:LEU:HD21 | 2:1758:A:CYS:HB3  | 16       | 0.35          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 1        | 0.35          |
| (2,1155) | 2:1743:A:VAL:HG21 | 2:1744:A:HIS:H    | 1        | 0.35          |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 2        | 0.35          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 8        | 0.35          |
| (2,1130) | 2:1761:A:MET:HE3  | 2:1739:A:ILE:HA   | 11       | 0.35          |
| (2,1085) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:H    | 10       | 0.35          |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD22 | 6        | 0.35          |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 1        | 0.35          |
| (2,997)  | 2:1733:A:LEU:HD13 | 2:1733:A:LEU:H    | 5        | 0.35          |
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 13       | 0.35          |
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 19       | 0.35          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 10       | 0.35          |
| (2,960)  | 2:1739:A:ILE:HD13 | 2:1735:A:ILE:HG22 | 20       | 0.35          |
| (2,923)  | 2:1765:A:VAL:HG23 | 2:1745:A:ALA:HB3  | 2        | 0.35          |
| (2,919)  | 2:1765:A:VAL:HG21 | 2:1762:A:LYS:HA   | 2        | 0.35          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 17       | 0.35          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 5        | 0.35          |
| (2,850)  | 2:1807:A:LEU:HD21 | 2:1801:A:CYS:HB3  | 13       | 0.35          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 2        | 0.35          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 3        | 0.35          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 16       | 0.35          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 11       | 0.35          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 16       | 0.35          |
| (2,661)  | 1:111:B:ALA:HB3   | 1:112:B:SER:HB3   | 5        | 0.35          |
| (2,612)  | 1:133:B:GLU:HG3   | 1:133:B:GLU:HA    | 18       | 0.35          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 11       | 0.35          |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD22  | 15       | 0.35          |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG21  | 8        | 0.35          |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG23  | 5        | 0.35          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 15       | 0.35          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 17       | 0.35          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 20       | 0.35          |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 12       | 0.35          |
| (2,387)  | 1:116:B:MET:H     | 1:115:B:GLN:HB2   | 15       | 0.35          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB3  | 7        | 0.35          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB2  | 17       | 0.35          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 14       | 0.35          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 2        | 0.35          |
| (2,94)   | 2:1786:A:ILE:H    | 2:1789:A:ALA:HB1  | 4        | 0.35          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 7        | 0.34          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 11       | 0.34          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 15       | 0.34          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 18       | 0.34          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 13       | 0.34          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 15       | 0.34          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 16       | 0.34          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 7        | 0.34          |
| (2,1551) | 2:1735:A:ILE:HG22 | 2:1791:A:TYR:HB2  | 5        | 0.34          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 17       | 0.34          |
| (2,1458) | 2:1803:A:VAL:HA   | 2:1803:A:VAL:HG23 | 14       | 0.34          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 13       | 0.34          |
| (2,1346) | 2:1755:A:LEU:HD23 | 2:1758:A:CYS:HB3  | 19       | 0.34          |
| (2,1346) | 2:1755:A:LEU:HD22 | 2:1758:A:CYS:HB3  | 20       | 0.34          |
| (2,1304) | 2:1751:A:ALA:HB1  | 2:1752:A:ASN:HB2  | 2        | 0.34          |
| (2,1290) | 2:1761:A:MET:HB2  | 2:1745:A:ALA:HB1  | 2        | 0.34          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 14       | 0.34          |
| (2,1150) | 2:1743:A:VAL:HG23 | 2:1803:A:VAL:HG11 | 1        | 0.34          |
| (2,1136) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:H    | 5        | 0.34          |
| (2,1130) | 2:1761:A:MET:HE2  | 2:1739:A:ILE:HA   | 6        | 0.34          |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 2        | 0.34          |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 3        | 0.34          |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 9        | 0.34          |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 11       | 0.34          |
| (2,1081) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HG   | 3        | 0.34          |
| (2,1081) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HG   | 16       | 0.34          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG21 | 17       | 0.34          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD23 | 18       | 0.34          |
| (2,1030) | 2:1807:A:LEU:HD12 | 2:1801:A:CYS:HB2  | 6        | 0.34          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 18       | 0.34          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 7        | 0.34          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 13       | 0.34          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 15       | 0.34          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 15       | 0.34          |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG22 | 18       | 0.34          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 19       | 0.34          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD12 | 6        | 0.34          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 12       | 0.34          |
| (2,919)  | 2:1765:A:VAL:HG23 | 2:1762:A:LYS:HA   | 14       | 0.34          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 14       | 0.34          |
| (2,869)  | 2:1747:A:GLN:HA   | 2:1747:A:GLN:HG2  | 13       | 0.34          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD13 | 3        | 0.34          |
| (2,850)  | 2:1807:A:LEU:HD23 | 2:1801:A:CYS:HB3  | 15       | 0.34          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 12       | 0.34          |
| (2,765)  | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:HE2  | 7        | 0.34          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 19       | 0.34          |
| (2,661)  | 1:111:B:ALA:HB1   | 1:112:B:SER:HB3   | 1        | 0.34          |
| (2,617)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:HA    | 1        | 0.34          |
| (2,558)  | 1:120:B:ILE:HD11  | 1:120:B:ILE:H     | 1        | 0.34          |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG22  | 12       | 0.34          |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 5        | 0.34          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG23  | 13       | 0.34          |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 4        | 0.34          |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 6        | 0.34          |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 12       | 0.34          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 6        | 0.34          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 15       | 0.34          |
| (2,247)  | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 19       | 0.34          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 12       | 0.34          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 15       | 0.34          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 18       | 0.34          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 18       | 0.34          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 5        | 0.34          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 6        | 0.33          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 3        | 0.33          |
| (2,1727) | 2:1781:A:ILE:HG23 | 2:1767:A:HIS:HD2  | 5        | 0.33          |
| (2,1727) | 2:1781:A:ILE:HG23 | 2:1767:A:HIS:HD2  | 18       | 0.33          |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG21 | 1        | 0.33          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 14       | 0.33          |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 1        | 0.33          |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 16       | 0.33          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD13 | 19       | 0.33          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 15       | 0.33          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 19       | 0.33          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 15       | 0.33          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD13 | 17       | 0.33          |
| (2,1415) | 2:1735:A:ILE:HD13 | 2:1735:A:ILE:H    | 10       | 0.33          |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG12 | 1        | 0.33          |
| (2,1346) | 2:1755:A:LEU:HD22 | 2:1758:A:CYS:HB3  | 7        | 0.33          |
| (2,1156) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HE22 | 11       | 0.33          |
| (2,1155) | 2:1743:A:VAL:HG22 | 2:1744:A:HIS:H    | 19       | 0.33          |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 19       | 0.33          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 17       | 0.33          |
| (2,1085) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:H    | 16       | 0.33          |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 17       | 0.33          |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD22 | 14       | 0.33          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 7        | 0.33          |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 15       | 0.33          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 6        | 0.33          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 16       | 0.33          |
| (2,951)  | 2:1780:A:PRO:HB3  | 1:134:B:ILE:HG22  | 7        | 0.33          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD13 | 4        | 0.33          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 15       | 0.33          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD22 | 11       | 0.33          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD21 | 12       | 0.33          |
| (2,914)  | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 6        | 0.33          |
| (2,889)  | 2:1741:A:SER:HB3  | 2:1761:A:MET:HG3  | 4        | 0.33          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG21 | 6        | 0.33          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 16       | 0.33          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD12 | 7        | 0.33          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 13       | 0.33          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 4        | 0.33          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 14       | 0.33          |
| (2,750)  | 2:1812:A:LYS:HG2  | 2:1812:A:LYS:H    | 10       | 0.33          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 1        | 0.33          |
| (2,685)  | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG2  | 9        | 0.33          |
| (2,668)  | 1:120:B:ILE:HD13  | 1:116:B:MET:HA    | 19       | 0.33          |
| (2,558)  | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 7        | 0.33          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 8        | 0.33          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 8        | 0.33          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 4        | 0.33          |
| (2,463)  | 1:134:B:ILE:HD11  | 1:134:B:ILE:H     | 5        | 0.33          |
| (2,463)  | 1:134:B:ILE:HD13  | 1:134:B:ILE:H     | 8        | 0.33          |
| (2,380)  | 1:132:B:GLU:H     | 1:132:B:GLU:HG2   | 17       | 0.33          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG22  | 19       | 0.33          |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 14       | 0.33          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 16       | 0.33          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 5        | 0.33          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 8        | 0.33          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 13       | 0.33          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 16       | 0.33          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 11       | 0.33          |
| (2,105)  | 2:1782:A:CYS:H    | 2:1781:A:ILE:HG12 | 12       | 0.33          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 9        | 0.33          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 10       | 0.33          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 13       | 0.33          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 16       | 0.33          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 19       | 0.32          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 20       | 0.32          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 7        | 0.32          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 19       | 0.32          |
| (2,1698) | 2:1788:A:LEU:HD21 | 2:1787:A:ALA:H    | 10       | 0.32          |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 15       | 0.32          |
| (2,1607) | 2:1781:A:ILE:HD12 | 2:1782:A:CYS:H    | 18       | 0.32          |
| (2,1530) | 2:1746:A:ALA:HB2  | 2:1802:A:PRO:HB2  | 9        | 0.32          |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 17       | 0.32          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 5        | 0.32          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 20       | 0.32          |
| (2,1358) | 2:1742:A:LEU:HD12 | 2:1803:A:VAL:HG11 | 6        | 0.32          |
| (2,1346) | 2:1755:A:LEU:HD23 | 2:1758:A:CYS:HB3  | 2        | 0.32          |
| (2,1331) | 2:1811:A:GLN:HB3  | 2:1811:A:GLN:H    | 9        | 0.32          |
| (2,1331) | 2:1811:A:GLN:HB3  | 2:1811:A:GLN:H    | 14       | 0.32          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 2        | 0.32          |
| (2,1184) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD3  | 12       | 0.32          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 2        | 0.32          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 7        | 0.32          |
| (2,1175) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:HA   | 9        | 0.32          |
| (2,1175) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:HA   | 15       | 0.32          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 19       | 0.32          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 15       | 0.32          |
| (2,1155) | 2:1743:A:VAL:HG21 | 2:1744:A:HIS:H    | 20       | 0.32          |
| (2,1153) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HG2  | 3        | 0.32          |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 5        | 0.32          |
| (2,1150) | 2:1743:A:VAL:HG21 | 2:1803:A:VAL:HG12 | 10       | 0.32          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG12 | 12       | 0.32          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 16       | 0.32          |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 1        | 0.32          |
| (2,1085) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:H    | 8        | 0.32          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD23 | 13       | 0.32          |
| (2,1081) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HG   | 11       | 0.32          |
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 4        | 0.32          |
| (2,997)  | 2:1733:A:LEU:HD12 | 2:1733:A:LEU:H    | 16       | 0.32          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG13 | 14       | 0.32          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 20       | 0.32          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 19       | 0.32          |
| (2,960)  | 2:1739:A:ILE:HD13 | 2:1735:A:ILE:HG23 | 10       | 0.32          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 17       | 0.32          |
| (2,923)  | 2:1765:A:VAL:HG21 | 2:1745:A:ALA:HB2  | 9        | 0.32          |
| (2,878)  | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 14       | 0.32          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG21 | 18       | 0.32          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 20       | 0.32          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 8        | 0.32          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 11       | 0.32          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 15       | 0.32          |
| (2,666)  | 1:120:B:ILE:HD13  | 1:117:B:ASP:HB3   | 15       | 0.32          |
| (2,661)  | 1:111:B:ALA:HB2   | 1:112:B:SER:HB3   | 7        | 0.32          |
| (2,661)  | 1:111:B:ALA:HB1   | 1:112:B:SER:HB3   | 8        | 0.32          |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1   | 2        | 0.32          |
| (2,617)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:HA    | 14       | 0.32          |
| (2,552)  | 1:123:B:ILE:H     | 1:123:B:ILE:HB    | 15       | 0.32          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 19       | 0.32          |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG21  | 12       | 0.32          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 14       | 0.32          |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 2        | 0.32          |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 13       | 0.32          |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 1        | 0.32          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 8        | 0.32          |
| (2,192)  | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG23  | 15       | 0.32          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 4        | 0.32          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 3        | 0.32          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 6        | 0.32          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 11       | 0.32          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 14       | 0.32          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 15       | 0.32          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 18       | 0.32          |
| (2,1737) | 2:1785:A:LEU:HD12 | 2:1767:A:HIS:HD2  | 12       | 0.31          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 18       | 0.31          |
| (2,1727) | 2:1781:A:ILE:HG22 | 2:1767:A:HIS:HD2  | 19       | 0.31          |
| (2,1718) | 2:1805:A:PHE:HE2  | 2:1785:A:LEU:HD21 | 7        | 0.31          |
| (2,1698) | 2:1788:A:LEU:HD23 | 2:1787:A:ALA:H    | 6        | 0.31          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1640) | 2:1807:A:LEU:HA   | 2:1810:A:LYS:HG3  | 6        | 0.31          |
| (2,1607) | 2:1781:A:ILE:HD13 | 2:1782:A:CYS:H    | 11       | 0.31          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 1        | 0.31          |
| (2,1515) | 2:1764:A:VAL:HG12 | 2:1761:A:MET:HG2  | 8        | 0.31          |
| (2,1506) | 2:1781:A:ILE:HD12 | 2:1781:A:ILE:H    | 16       | 0.31          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 2        | 0.31          |
| (2,1435) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:HD12 | 15       | 0.31          |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 5        | 0.31          |
| (2,1387) | 2:1785:A:LEU:HD13 | 2:1805:A:PHE:HE1  | 16       | 0.31          |
| (2,1358) | 2:1742:A:LEU:HD11 | 2:1803:A:VAL:HG13 | 12       | 0.31          |
| (2,1346) | 2:1755:A:LEU:HD22 | 2:1758:A:CYS:HB3  | 18       | 0.31          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 8        | 0.31          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 17       | 0.31          |
| (2,1244) | 2:1775:A:THR:HG21 | 2:1776:A:ASN:HB2  | 9        | 0.31          |
| (2,1244) | 2:1775:A:THR:HG23 | 2:1776:A:ASN:HB2  | 13       | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 6        | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 10       | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 11       | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 14       | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 15       | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 18       | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 19       | 0.31          |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 20       | 0.31          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 13       | 0.31          |
| (2,1175) | 2:1755:A:LEU:HD11 | 2:1755:A:LEU:HA   | 16       | 0.31          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 18       | 0.31          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 18       | 0.31          |
| (2,1153) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HG2  | 2        | 0.31          |
| (2,1150) | 2:1743:A:VAL:HG23 | 2:1803:A:VAL:HG13 | 11       | 0.31          |
| (2,1136) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:H    | 14       | 0.31          |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 16       | 0.31          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 1        | 0.31          |
| (2,1130) | 2:1761:A:MET:HE2  | 2:1739:A:ILE:HA   | 3        | 0.31          |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD21 | 9        | 0.31          |
| (2,1069) | 2:1768:A:THR:HG21 | 2:1785:A:LEU:HD23 | 4        | 0.31          |
| (2,1030) | 2:1807:A:LEU:HD13 | 2:1801:A:CYS:HB2  | 15       | 0.31          |
| (2,987)  | 2:1764:A:VAL:HA   | 2:1781:A:ILE:HG23 | 7        | 0.31          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 11       | 0.31          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 10       | 0.31          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD12 | 13       | 0.31          |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG23 | 17       | 0.31          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD13 | 13       | 0.31          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD13 | 20       | 0.31          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 15       | 0.31          |
| (2,923)  | 2:1765:A:VAL:HG21 | 2:1745:A:ALA:HB3  | 12       | 0.31          |
| (2,919)  | 2:1765:A:VAL:HG21 | 2:1762:A:LYS:HA   | 4        | 0.31          |
| (2,914)  | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 20       | 0.31          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 2        | 0.31          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 10       | 0.31          |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 1        | 0.31          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 14       | 0.31          |
| (2,754)  | 2:1774:A:LYS:HG2  | 2:1774:A:LYS:HE3  | 19       | 0.31          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD22 | 8        | 0.31          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 2        | 0.31          |
| (2,647)  | 1:133:B:GLU:HB3   | 1:131:B:ASN:HD22  | 19       | 0.31          |
| (2,617)  | 1:137:B:LEU:HD23  | 1:137:B:LEU:HA    | 7        | 0.31          |
| (2,617)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:HA    | 11       | 0.31          |
| (2,617)  | 1:137:B:LEU:HD22  | 1:137:B:LEU:HA    | 17       | 0.31          |
| (2,576)  | 1:119:B:VAL:HG11  | 1:120:B:ILE:H     | 18       | 0.31          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 2        | 0.31          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG22  | 9        | 0.31          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG23  | 17       | 0.31          |
| (2,517)  | 1:137:B:LEU:HB3   | 1:137:B:LEU:HD21  | 18       | 0.31          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 8        | 0.31          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 11       | 0.31          |
| (2,429)  | 1:125:B:SER:H     | 1:125:B:SER:HB2   | 11       | 0.31          |
| (2,429)  | 1:125:B:SER:H     | 1:125:B:SER:HB2   | 14       | 0.31          |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 10       | 0.31          |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 1        | 0.31          |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 18       | 0.31          |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 8        | 0.31          |
| (2,273)  | 2:1755:A:LEU:H    | 2:1758:A:CYS:HB2  | 10       | 0.31          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 8        | 0.31          |
| (2,210)  | 2:1739:A:ILE:HG23 | 2:1739:A:ILE:H    | 6        | 0.31          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 8        | 0.31          |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 13       | 0.31          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 16       | 0.31          |
| (2,131)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HG3  | 18       | 0.31          |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 1        | 0.31          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 19       | 0.31          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 18       | 0.3           |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 13       | 0.3           |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 17       | 0.3           |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 8        | 0.3           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 15       | 0.3           |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 18       | 0.3           |
| (2,1655) | 2:1787:A:ALA:HB1  | 2:1784:A:GLN:HB3  | 7        | 0.3           |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 15       | 0.3           |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE1  | 8        | 0.3           |
| (2,1555) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HD2   | 17       | 0.3           |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 9        | 0.3           |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 1        | 0.3           |
| (2,1529) | 2:1746:A:ALA:HB3  | 2:1747:A:GLN:HG3  | 11       | 0.3           |
| (2,1515) | 2:1764:A:VAL:HG12 | 2:1761:A:MET:HG2  | 9        | 0.3           |
| (2,1387) | 2:1785:A:LEU:HD11 | 2:1805:A:PHE:HE1  | 2        | 0.3           |
| (2,1358) | 2:1742:A:LEU:HD13 | 2:1803:A:VAL:HG12 | 3        | 0.3           |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 1        | 0.3           |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 4        | 0.3           |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 6        | 0.3           |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 10       | 0.3           |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 18       | 0.3           |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 4        | 0.3           |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 11       | 0.3           |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 7        | 0.3           |
| (2,1215) | 2:1740:A:GLN:HG2  | 2:1740:A:GLN:HE22 | 12       | 0.3           |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 1        | 0.3           |
| (2,1175) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:HA   | 11       | 0.3           |
| (2,1175) | 2:1755:A:LEU:HD11 | 2:1755:A:LEU:HA   | 20       | 0.3           |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 12       | 0.3           |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 7        | 0.3           |
| (2,1089) | 2:1774:A:LYS:HA   | 2:1779:A:CYS:HB2  | 19       | 0.3           |
| (2,1030) | 2:1807:A:LEU:HD12 | 2:1801:A:CYS:HB2  | 5        | 0.3           |
| (2,997)  | 2:1733:A:LEU:HD11 | 2:1733:A:LEU:H    | 2        | 0.3           |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 9        | 0.3           |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 17       | 0.3           |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG23 | 3        | 0.3           |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 3        | 0.3           |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 5        | 0.3           |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD12 | 11       | 0.3           |
| (2,923)  | 2:1765:A:VAL:HG23 | 2:1745:A:ALA:HB1  | 15       | 0.3           |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 3        | 0.3           |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 17       | 0.3           |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 19       | 0.3           |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 20       | 0.3           |
| (2,685)  | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG2  | 14       | 0.3           |
| (2,676)  | 1:132:B:GLU:HG2   | 1:135:B:LEU:HB2   | 5        | 0.3           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,622)  | 1:139:B:ASP:HB3   | 1:140:B:PRO:HD2   | 2        | 0.3           |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 2        | 0.3           |
| (2,472)  | 1:123:B:ILE:H     | 1:123:B:ILE:HD11  | 15       | 0.3           |
| (2,463)  | 1:134:B:ILE:HD12  | 1:134:B:ILE:H     | 7        | 0.3           |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 15       | 0.3           |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB3  | 10       | 0.3           |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB3  | 12       | 0.3           |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 12       | 0.3           |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 4        | 0.3           |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 9        | 0.3           |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 11       | 0.3           |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 14       | 0.3           |
| (2,15)   | 2:1752:A:ASN:HB3  | 2:1752:A:ASN:HD22 | 7        | 0.3           |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 6        | 0.3           |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 13       | 0.29          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 4        | 0.29          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 6        | 0.29          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 14       | 0.29          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 17       | 0.29          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 19       | 0.29          |
| (2,1737) | 2:1785:A:LEU:HD11 | 2:1767:A:HIS:HD2  | 2        | 0.29          |
| (2,1737) | 2:1785:A:LEU:HD11 | 2:1767:A:HIS:HD2  | 11       | 0.29          |
| (2,1699) | 2:1781:A:ILE:HD11 | 2:1767:A:HIS:HD2  | 10       | 0.29          |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE2  | 1        | 0.29          |
| (2,1529) | 2:1746:A:ALA:HB3  | 2:1747:A:GLN:HG3  | 4        | 0.29          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 10       | 0.29          |
| (2,1528) | 2:1747:A:GLN:HG2  | 2:1746:A:ALA:HB3  | 13       | 0.29          |
| (2,1506) | 2:1781:A:ILE:HD11 | 2:1781:A:ILE:H    | 9        | 0.29          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 12       | 0.29          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 16       | 0.29          |
| (2,1415) | 2:1735:A:ILE:HD11 | 2:1735:A:ILE:H    | 11       | 0.29          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 17       | 0.29          |
| (2,1346) | 2:1755:A:LEU:HD21 | 2:1758:A:CYS:HB3  | 13       | 0.29          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 12       | 0.29          |
| (2,1304) | 2:1751:A:ALA:HB1  | 2:1752:A:ASN:HB2  | 19       | 0.29          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 1        | 0.29          |
| (2,1184) | 2:1803:A:VAL:HG11 | 2:1804:A:PRO:HD3  | 6        | 0.29          |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 15       | 0.29          |
| (2,1175) | 2:1755:A:LEU:HD11 | 2:1755:A:LEU:HA   | 3        | 0.29          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 5        | 0.29          |
| (2,1155) | 2:1743:A:VAL:HG21 | 2:1744:A:HIS:H    | 11       | 0.29          |
| (2,1148) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HD2   | 10       | 0.29          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 1        | 0.29          |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 17       | 0.29          |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 20       | 0.29          |
| (2,1130) | 2:1761:A:MET:HE1  | 2:1739:A:ILE:HA   | 4        | 0.29          |
| (2,1093) | 2:1774:A:LYS:HA   | 2:1774:A:LYS:HG3  | 18       | 0.29          |
| (2,1083) | 2:1781:A:ILE:HG23 | 2:1785:A:LEU:HD21 | 4        | 0.29          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG23 | 8        | 0.29          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG23 | 10       | 0.29          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 17       | 0.29          |
| (2,1034) | 2:1735:A:ILE:HG21 | 2:1739:A:ILE:HB   | 5        | 0.29          |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 7        | 0.29          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 10       | 0.29          |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 11       | 0.29          |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 15       | 0.29          |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 18       | 0.29          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 4        | 0.29          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG13 | 8        | 0.29          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD13 | 10       | 0.29          |
| (2,923)  | 2:1765:A:VAL:HG23 | 2:1745:A:ALA:HB1  | 4        | 0.29          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 11       | 0.29          |
| (2,862)  | 2:1731:A:ARG:HG3  | 2:1735:A:ILE:HD11 | 18       | 0.29          |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 18       | 0.29          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 13       | 0.29          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 15       | 0.29          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 10       | 0.29          |
| (2,754)  | 2:1774:A:LYS:HG2  | 2:1774:A:LYS:HE3  | 9        | 0.29          |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 13       | 0.29          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 12       | 0.29          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 20       | 0.29          |
| (2,463)  | 1:134:B:ILE:HD11  | 1:134:B:ILE:H     | 4        | 0.29          |
| (2,386)  | 1:126:B:LEU:H     | 1:126:B:LEU:HD12  | 16       | 0.29          |
| (2,359)  | 1:121:B:ASP:H     | 1:120:B:ILE:HG22  | 11       | 0.29          |
| (2,345)  | 1:130:B:TYR:H     | 1:129:B:SER:HB3   | 13       | 0.29          |
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 13       | 0.29          |
| (2,290)  | 2:1773:A:ARG:H    | 2:1773:A:ARG:HG2  | 17       | 0.29          |
| (2,277)  | 2:1738:A:ALA:H    | 2:1737:A:ARG:HD2  | 11       | 0.29          |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 4        | 0.29          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 16       | 0.29          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 17       | 0.29          |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 20       | 0.29          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 3        | 0.29          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 10       | 0.29          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 11       | 0.29          |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 10       | 0.29          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 3        | 0.29          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 14       | 0.29          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD21 | 20       | 0.29          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 2        | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 3        | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 4        | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 5        | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 6        | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 14       | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 18       | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 19       | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 20       | 0.28          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 10       | 0.28          |
| (2,1737) | 2:1785:A:LEU:HD13 | 2:1767:A:HIS:HD2  | 3        | 0.28          |
| (2,1677) | 2:1767:A:HIS:HB3  | 2:1781:A:ILE:HG23 | 7        | 0.28          |
| (2,1662) | 2:1768:A:THR:HG21 | 2:1805:A:PHE:HD1  | 5        | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 3        | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 4        | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 5        | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 7        | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 8        | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 9        | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 10       | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 11       | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 12       | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 13       | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 17       | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 19       | 0.28          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 20       | 0.28          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 15       | 0.28          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 7        | 0.28          |
| (2,1529) | 2:1746:A:ALA:HB1  | 2:1747:A:GLN:HG3  | 20       | 0.28          |
| (2,1506) | 2:1781:A:ILE:HD12 | 2:1781:A:ILE:H    | 3        | 0.28          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 8        | 0.28          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 15       | 0.28          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 1        | 0.28          |
| (2,1414) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HB3   | 19       | 0.28          |
| (2,1385) | 2:1785:A:LEU:HD12 | 2:1768:A:THR:HG23 | 12       | 0.28          |
| (2,1379) | 2:1809:A:ILE:HG23 | 2:1793:A:ALA:HB2  | 4        | 0.28          |
| (2,1379) | 2:1809:A:ILE:HG21 | 2:1793:A:ALA:HB2  | 5        | 0.28          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 14       | 0.28          |
| (2,1304) | 2:1751:A:ALA:HB1  | 2:1752:A:ASN:HB2  | 7        | 0.28          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG11 | 11       | 0.28          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 8        | 0.28          |
| (2,1184) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD3  | 5        | 0.28          |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 14       | 0.28          |
| (2,1146) | 2:1788:A:LEU:HD22 | 2:1735:A:ILE:HA   | 10       | 0.28          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG22 | 6        | 0.28          |
| (2,1069) | 2:1768:A:THR:HG22 | 2:1785:A:LEU:HD22 | 17       | 0.28          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 20       | 0.28          |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 17       | 0.28          |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 12       | 0.28          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 13       | 0.28          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 17       | 0.28          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 14       | 0.28          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG13 | 9        | 0.28          |
| (2,960)  | 2:1739:A:ILE:HD13 | 2:1735:A:ILE:HG23 | 1        | 0.28          |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG22 | 15       | 0.28          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD13 | 1        | 0.28          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 19       | 0.28          |
| (2,923)  | 2:1765:A:VAL:HG21 | 2:1745:A:ALA:HB2  | 19       | 0.28          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG22 | 7        | 0.28          |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 3        | 0.28          |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 12       | 0.28          |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 13       | 0.28          |
| (2,860)  | 2:1747:A:GLN:HG3  | 2:1747:A:GLN:HE22 | 15       | 0.28          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 18       | 0.28          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 19       | 0.28          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 17       | 0.28          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 2        | 0.28          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 16       | 0.28          |
| (2,761)  | 2:1812:A:LYS:HB3  | 2:1812:A:LYS:H    | 13       | 0.28          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 3        | 0.28          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 14       | 0.28          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 20       | 0.28          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD22 | 6        | 0.28          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 12       | 0.28          |
| (2,685)  | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG2  | 10       | 0.28          |
| (2,657)  | 1:135:B:LEU:HD22  | 1:130:B:TYR:HD1   | 10       | 0.28          |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1   | 19       | 0.28          |
| (2,636)  | 1:135:B:LEU:HD21  | 1:132:B:GLU:HB2   | 3        | 0.28          |
| (2,576)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:H     | 1        | 0.28          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,540)  | 1:134:B:ILE:HG21  | 2:1781:A:ILE:HA   | 20       | 0.28          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 11       | 0.28          |
| (2,345)  | 1:130:B:TYR:H     | 1:129:B:SER:HB3   | 12       | 0.28          |
| (2,345)  | 1:130:B:TYR:H     | 1:129:B:SER:HB3   | 14       | 0.28          |
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 9        | 0.28          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 7        | 0.28          |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 11       | 0.28          |
| (2,210)  | 2:1739:A:ILE:HG23 | 2:1739:A:ILE:H    | 19       | 0.28          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 2        | 0.28          |
| (2,196)  | 2:1760:A:LYS:HG3  | 2:1761:A:MET:H    | 20       | 0.28          |
| (2,158)  | 2:1798:A:GLU:H    | 2:1798:A:GLU:HB3  | 13       | 0.28          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD21 | 13       | 0.28          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 1        | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 7        | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 8        | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 9        | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 10       | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 11       | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 12       | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 15       | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 16       | 0.27          |
| (3,34)   | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HB2  | 17       | 0.27          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 8        | 0.27          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 1        | 0.27          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD1  | 5        | 0.27          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 7        | 0.27          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 9        | 0.27          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 11       | 0.27          |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG22 | 3        | 0.27          |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG23 | 12       | 0.27          |
| (2,1677) | 2:1767:A:HIS:HB3  | 2:1781:A:ILE:HG23 | 20       | 0.27          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 1        | 0.27          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 2        | 0.27          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 6        | 0.27          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 14       | 0.27          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 15       | 0.27          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 16       | 0.27          |
| (2,1628) | 2:1740:A:GLN:HB3  | 2:1740:A:GLN:HG3  | 18       | 0.27          |
| (2,1572) | 2:1809:A:ILE:HD13 | 2:1805:A:PHE:HD2  | 14       | 0.27          |
| (2,1529) | 2:1746:A:ALA:HB3  | 2:1747:A:GLN:HG3  | 2        | 0.27          |
| (2,1529) | 2:1746:A:ALA:HB3  | 2:1747:A:GLN:HG3  | 8        | 0.27          |
| (2,1529) | 2:1746:A:ALA:HB2  | 2:1747:A:GLN:HG3  | 9        | 0.27          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG23 | 15       | 0.27          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 1        | 0.27          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 2        | 0.27          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 3        | 0.27          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG21 | 6        | 0.27          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 17       | 0.27          |
| (2,1387) | 2:1785:A:LEU:HD11 | 2:1805:A:PHE:HE2  | 11       | 0.27          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG22 | 3        | 0.27          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG22 | 12       | 0.27          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG23 | 19       | 0.27          |
| (2,1371) | 2:1764:A:VAL:HG22 | 2:1764:A:VAL:H    | 18       | 0.27          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG13 | 3        | 0.27          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG12 | 8        | 0.27          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG11 | 12       | 0.27          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 1        | 0.27          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 15       | 0.27          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 19       | 0.27          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 10       | 0.27          |
| (2,1184) | 2:1803:A:VAL:HG12 | 2:1804:A:PRO:HD3  | 3        | 0.27          |
| (2,1184) | 2:1803:A:VAL:HG13 | 2:1804:A:PRO:HD3  | 8        | 0.27          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 8        | 0.27          |
| (2,1156) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HE22 | 13       | 0.27          |
| (2,1155) | 2:1743:A:VAL:HG22 | 2:1744:A:HIS:H    | 3        | 0.27          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 9        | 0.27          |
| (2,1155) | 2:1743:A:VAL:HG22 | 2:1744:A:HIS:H    | 10       | 0.27          |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 3        | 0.27          |
| (2,1136) | 2:1765:A:VAL:HG13 | 2:1766:A:GLN:H    | 4        | 0.27          |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 8        | 0.27          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG22 | 7        | 0.27          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 1        | 0.27          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 11       | 0.27          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 18       | 0.27          |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 3        | 0.27          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 3        | 0.27          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 6        | 0.27          |
| (2,1034) | 2:1735:A:ILE:HG21 | 2:1739:A:ILE:HB   | 14       | 0.27          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 19       | 0.27          |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 20       | 0.27          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 2        | 0.27          |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 9        | 0.27          |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG22 | 9        | 0.27          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 20       | 0.27          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 5        | 0.27          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 1        | 0.27          |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 9        | 0.27          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 13       | 0.27          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 5        | 0.27          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 18       | 0.27          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 13       | 0.27          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 3        | 0.27          |
| (2,636)  | 1:135:B:LEU:HD21  | 1:132:B:GLU:HB2   | 10       | 0.27          |
| (2,576)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:H     | 4        | 0.27          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD11  | 6        | 0.27          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD12  | 9        | 0.27          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG23  | 7        | 0.27          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG21  | 13       | 0.27          |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG21  | 7        | 0.27          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 2        | 0.27          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 14       | 0.27          |
| (2,427)  | 1:136:B:GLY:H     | 1:135:B:LEU:HG    | 20       | 0.27          |
| (2,345)  | 1:130:B:TYR:H     | 1:129:B:SER:HB3   | 2        | 0.27          |
| (2,345)  | 1:130:B:TYR:H     | 1:129:B:SER:HB3   | 20       | 0.27          |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 5        | 0.27          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB2  | 14       | 0.27          |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 10       | 0.27          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 15       | 0.27          |
| (2,210)  | 2:1739:A:ILE:HG23 | 2:1739:A:ILE:H    | 18       | 0.27          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 6        | 0.27          |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 19       | 0.27          |
| (2,119)  | 2:1752:A:ASN:HB2  | 2:1752:A:ASN:H    | 20       | 0.27          |
| (3,36)   | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG3  | 1        | 0.26          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 9        | 0.26          |
| (2,1741) | 2:1795:A:HIS:HB3  | 2:1795:A:HIS:HD2  | 9        | 0.26          |
| (2,1727) | 2:1781:A:ILE:HG23 | 2:1767:A:HIS:HD2  | 6        | 0.26          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 7        | 0.26          |
| (2,1644) | 2:1737:A:ARG:HB3  | 2:1738:A:ALA:H    | 20       | 0.26          |
| (2,1506) | 2:1781:A:ILE:HD12 | 2:1781:A:ILE:H    | 2        | 0.26          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 7        | 0.26          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG21 | 9        | 0.26          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 10       | 0.26          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 11       | 0.26          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 14       | 0.26          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 18       | 0.26          |
| (2,1451) | 2:1789:A:ALA:HB2  | 2:1805:A:PHE:HD1  | 19       | 0.26          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1387) | 2:1785:A:LEU:HD11 | 2:1805:A:PHE:HE1  | 1        | 0.26          |
| (2,1387) | 2:1785:A:LEU:HD12 | 2:1805:A:PHE:HE2  | 18       | 0.26          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 2        | 0.26          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 11       | 0.26          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 15       | 0.26          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG23 | 20       | 0.26          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 15       | 0.26          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 18       | 0.26          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 11       | 0.26          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG11 | 17       | 0.26          |
| (2,1244) | 2:1775:A:THR:HG21 | 2:1776:A:ASN:HB2  | 4        | 0.26          |
| (2,1244) | 2:1775:A:THR:HG22 | 2:1776:A:ASN:HB2  | 19       | 0.26          |
| (2,1156) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HE22 | 17       | 0.26          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 5        | 0.26          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 17       | 0.26          |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 18       | 0.26          |
| (2,1130) | 2:1761:A:MET:HE2  | 2:1739:A:ILE:HA   | 5        | 0.26          |
| (2,1127) | 2:1761:A:MET:HE3  | 2:1738:A:ALA:HB3  | 4        | 0.26          |
| (2,1119) | 2:1739:A:ILE:HG23 | 2:1736:A:GLN:HA   | 13       | 0.26          |
| (2,1083) | 2:1781:A:ILE:HG22 | 2:1785:A:LEU:HD22 | 7        | 0.26          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG22 | 13       | 0.26          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 19       | 0.26          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 4        | 0.26          |
| (2,1043) | 2:1782:A:CYS:HA   | 2:1785:A:LEU:HD23 | 15       | 0.26          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 4        | 0.26          |
| (2,1034) | 2:1735:A:ILE:HG22 | 2:1739:A:ILE:HB   | 9        | 0.26          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 5        | 0.26          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 1        | 0.26          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG13 | 5        | 0.26          |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG23 | 4        | 0.26          |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG22 | 7        | 0.26          |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG21 | 14       | 0.26          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 9        | 0.26          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 14       | 0.26          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 16       | 0.26          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD12 | 18       | 0.26          |
| (2,878)  | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 18       | 0.26          |
| (2,874)  | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 12       | 0.26          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 9        | 0.26          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 3        | 0.26          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 8        | 0.26          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 10       | 0.26          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 8        | 0.26          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 9        | 0.26          |
| (2,754)  | 2:1774:A:LYS:HG2  | 2:1774:A:LYS:HE3  | 12       | 0.26          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 1        | 0.26          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 2        | 0.26          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 4        | 0.26          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 13       | 0.26          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 8        | 0.26          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 19       | 0.26          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 20       | 0.26          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 6        | 0.26          |
| (2,668)  | 1:120:B:ILE:HD12  | 1:116:B:MET:HA    | 3        | 0.26          |
| (2,661)  | 1:111:B:ALA:HB3   | 1:112:B:SER:HB3   | 4        | 0.26          |
| (2,540)  | 1:134:B:ILE:HG22  | 2:1781:A:ILE:HA   | 8        | 0.26          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 3        | 0.26          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 17       | 0.26          |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 14       | 0.26          |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 16       | 0.26          |
| (2,293)  | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 17       | 0.26          |
| (2,210)  | 2:1739:A:ILE:HG23 | 2:1739:A:ILE:H    | 1        | 0.26          |
| (2,210)  | 2:1739:A:ILE:HG22 | 2:1739:A:ILE:H    | 2        | 0.26          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 3        | 0.26          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 14       | 0.26          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 13       | 0.26          |
| (2,114)  | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 9        | 0.26          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD23 | 7        | 0.26          |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD21 | 14       | 0.25          |
| (2,1718) | 2:1805:A:PHE:HE1  | 2:1785:A:LEU:HD22 | 20       | 0.25          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 3        | 0.25          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 4        | 0.25          |
| (2,1698) | 2:1788:A:LEU:HD21 | 2:1787:A:ALA:H    | 13       | 0.25          |
| (2,1698) | 2:1788:A:LEU:HD21 | 2:1787:A:ALA:H    | 17       | 0.25          |
| (2,1670) | 2:1774:A:LYS:HG3  | 2:1779:A:CYS:HB2  | 20       | 0.25          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB1  | 13       | 0.25          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 3        | 0.25          |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE2   | 2        | 0.25          |
| (2,1551) | 2:1735:A:ILE:HG22 | 2:1791:A:TYR:HB2  | 14       | 0.25          |
| (2,1551) | 2:1735:A:ILE:HG23 | 2:1791:A:TYR:HB2  | 15       | 0.25          |
| (2,1529) | 2:1746:A:ALA:HB3  | 2:1747:A:GLN:HG3  | 5        | 0.25          |
| (2,1529) | 2:1746:A:ALA:HB2  | 2:1747:A:GLN:HG3  | 6        | 0.25          |
| (2,1506) | 2:1781:A:ILE:HD11 | 2:1781:A:ILE:H    | 1        | 0.25          |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 4        | 0.25          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD13 | 6        | 0.25          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD11 | 7        | 0.25          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD12 | 13       | 0.25          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 20       | 0.25          |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 16       | 0.25          |
| (2,1397) | 2:1793:A:ALA:HB3  | 2:1794:A:LYS:H    | 5        | 0.25          |
| (2,1397) | 2:1793:A:ALA:HB2  | 2:1794:A:LYS:H    | 20       | 0.25          |
| (2,1387) | 2:1785:A:LEU:HD13 | 2:1805:A:PHE:HE2  | 3        | 0.25          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG23 | 1        | 0.25          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 4        | 0.25          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG23 | 7        | 0.25          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG22 | 8        | 0.25          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 18       | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 1        | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 2        | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 4        | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 5        | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 7        | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 12       | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 15       | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 16       | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 19       | 0.25          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 20       | 0.25          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG13 | 1        | 0.25          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 17       | 0.25          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 7        | 0.25          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 4        | 0.25          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 10       | 0.25          |
| (2,1156) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HE22 | 10       | 0.25          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 8        | 0.25          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 17       | 0.25          |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD21 | 8        | 0.25          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG23 | 14       | 0.25          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG21 | 20       | 0.25          |
| (2,1069) | 2:1768:A:THR:HG23 | 2:1785:A:LEU:HD23 | 9        | 0.25          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 5        | 0.25          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 12       | 0.25          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 14       | 0.25          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 3        | 0.25          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 1        | 0.25          |
| (2,1030) | 2:1807:A:LEU:HD12 | 2:1801:A:CYS:HB2  | 18       | 0.25          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 3        | 0.25          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (2,986) | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 12       | 0.25          |
| (2,980) | 2:1730:A:SER:HA   | 2:1733:A:LEU:HG   | 3        | 0.25          |
| (2,960) | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG21 | 2        | 0.25          |
| (2,937) | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD12 | 8        | 0.25          |
| (2,874) | 2:1792:A:HIS:HA   | 2:1739:A:ILE:HG23 | 4        | 0.25          |
| (2,855) | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 2        | 0.25          |
| (2,855) | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 3        | 0.25          |
| (2,855) | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 10       | 0.25          |
| (2,855) | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 12       | 0.25          |
| (2,855) | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 19       | 0.25          |
| (2,836) | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 1        | 0.25          |
| (2,836) | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 16       | 0.25          |
| (2,806) | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 10       | 0.25          |
| (2,806) | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 18       | 0.25          |
| (2,805) | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 8        | 0.25          |
| (2,805) | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 10       | 0.25          |
| (2,805) | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 16       | 0.25          |
| (2,743) | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 10       | 0.25          |
| (2,743) | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 20       | 0.25          |
| (2,732) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 2        | 0.25          |
| (2,732) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 3        | 0.25          |
| (2,732) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 4        | 0.25          |
| (2,731) | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 3        | 0.25          |
| (2,731) | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 10       | 0.25          |
| (2,731) | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 11       | 0.25          |
| (2,731) | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 15       | 0.25          |
| (2,722) | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD21 | 15       | 0.25          |
| (2,617) | 1:137:B:LEU:HD21  | 1:137:B:LEU:HA    | 12       | 0.25          |
| (2,576) | 1:119:B:VAL:HG12  | 1:120:B:ILE:H     | 2        | 0.25          |
| (2,576) | 1:119:B:VAL:HG11  | 1:120:B:ILE:H     | 14       | 0.25          |
| (2,558) | 1:120:B:ILE:HD13  | 1:120:B:ILE:H     | 8        | 0.25          |
| (2,540) | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 14       | 0.25          |
| (2,540) | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 19       | 0.25          |
| (2,519) | 1:125:B:SER:HB2   | 1:124:B:ILE:HG23  | 19       | 0.25          |
| (2,510) | 1:117:B:ASP:HA    | 1:119:B:VAL:HG21  | 5        | 0.25          |
| (2,397) | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 6        | 0.25          |
| (2,394) | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 3        | 0.25          |
| (2,394) | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 10       | 0.25          |
| (2,386) | 1:126:B:LEU:H     | 1:126:B:LEU:HD13  | 14       | 0.25          |
| (2,293) | 2:1736:A:GLN:HE22 | 2:1736:A:GLN:HA   | 8        | 0.25          |
| (2,289) | 2:1784:A:GLN:HE21 | 2:1784:A:GLN:HB3  | 12       | 0.25          |
| (2,247) | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 18       | 0.25          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,231)  | 2:1732:A:ARG:H    | 2:1731:A:ARG:HD2  | 14       | 0.25          |
| (2,210)  | 2:1739:A:ILE:HG21 | 2:1739:A:ILE:H    | 5        | 0.25          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 1        | 0.25          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 17       | 0.25          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 19       | 0.25          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 20       | 0.25          |
| (3,36)   | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG3  | 2        | 0.24          |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 2        | 0.24          |
| (2,1727) | 2:1781:A:ILE:HG21 | 2:1767:A:HIS:HD2  | 13       | 0.24          |
| (2,1727) | 2:1781:A:ILE:HG22 | 2:1767:A:HIS:HD2  | 20       | 0.24          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 1        | 0.24          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 2        | 0.24          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 6        | 0.24          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 8        | 0.24          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 9        | 0.24          |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG23 | 15       | 0.24          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB2  | 18       | 0.24          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 14       | 0.24          |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 17       | 0.24          |
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG23 | 6        | 0.24          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG21 | 4        | 0.24          |
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD2  | 6        | 0.24          |
| (2,1414) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HB3   | 15       | 0.24          |
| (2,1397) | 2:1793:A:ALA:HB2  | 2:1794:A:LYS:H    | 1        | 0.24          |
| (2,1387) | 2:1785:A:LEU:HD12 | 2:1805:A:PHE:HE1  | 12       | 0.24          |
| (2,1379) | 2:1809:A:ILE:HG23 | 2:1793:A:ALA:HB1  | 11       | 0.24          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG22 | 5        | 0.24          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 10       | 0.24          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 14       | 0.24          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG23 | 16       | 0.24          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 18       | 0.24          |
| (2,1368) | 2:1764:A:VAL:HG22 | 2:1781:A:ILE:HG23 | 19       | 0.24          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 3        | 0.24          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 3        | 0.24          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 6        | 0.24          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 8        | 0.24          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 10       | 0.24          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 11       | 0.24          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 13       | 0.24          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 14       | 0.24          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 1        | 0.24          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 3        | 0.24          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 4        | 0.24          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 17       | 0.24          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG12 | 5        | 0.24          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 2        | 0.24          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 4        | 0.24          |
| (2,1155) | 2:1743:A:VAL:HG22 | 2:1744:A:HIS:H    | 7        | 0.24          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG11 | 15       | 0.24          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG11 | 18       | 0.24          |
| (2,1146) | 2:1788:A:LEU:HD21 | 2:1735:A:ILE:HA   | 19       | 0.24          |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 12       | 0.24          |
| (2,1127) | 2:1761:A:MET:HE1  | 2:1738:A:ALA:HB3  | 20       | 0.24          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG22 | 9        | 0.24          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG22 | 19       | 0.24          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 2        | 0.24          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 3        | 0.24          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 9        | 0.24          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 10       | 0.24          |
| (2,1055) | 2:1780:A:PRO:HA   | 1:134:B:ILE:HG21  | 2        | 0.24          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 1        | 0.24          |
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 9        | 0.24          |
| (2,1034) | 2:1735:A:ILE:HG23 | 2:1739:A:ILE:HB   | 8        | 0.24          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 12       | 0.24          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 15       | 0.24          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 19       | 0.24          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 20       | 0.24          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 16       | 0.24          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 19       | 0.24          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 11       | 0.24          |
| (2,937)  | 2:1736:A:GLN:HA   | 2:1739:A:ILE:HD11 | 2        | 0.24          |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB1  | 3        | 0.24          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD12 | 5        | 0.24          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 6        | 0.24          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 16       | 0.24          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 4        | 0.24          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 9        | 0.24          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 17       | 0.24          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 9        | 0.24          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 12       | 0.24          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 6        | 0.24          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 4        | 0.24          |
| (2,750)  | 2:1812:A:LYS:HG2  | 2:1812:A:LYS:H    | 18       | 0.24          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 1        | 0.24          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 6        | 0.24          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 9        | 0.24          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 16       | 0.24          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 17       | 0.24          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 18       | 0.24          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 5        | 0.24          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 6        | 0.24          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 8        | 0.24          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 9        | 0.24          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 16       | 0.24          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 17       | 0.24          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 18       | 0.24          |
| (2,678)  | 1:134:B:ILE:HG22  | 1:131:B:ASN:HD22  | 9        | 0.24          |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1   | 18       | 0.24          |
| (2,622)  | 1:139:B:ASP:HB3   | 1:140:B:PRO:HD2   | 15       | 0.24          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 3        | 0.24          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 10       | 0.24          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG22  | 14       | 0.24          |
| (2,463)  | 1:134:B:ILE:HD11  | 1:134:B:ILE:H     | 9        | 0.24          |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 16       | 0.24          |
| (2,397)  | 1:139:B:ASP:H     | 1:139:B:ASP:HB2   | 17       | 0.24          |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 19       | 0.24          |
| (2,387)  | 1:116:B:MET:H     | 1:115:B:GLN:HB2   | 9        | 0.24          |
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 11       | 0.24          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 11       | 0.23          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 20       | 0.23          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 13       | 0.23          |
| (2,1727) | 2:1781:A:ILE:HG22 | 2:1767:A:HIS:HD2  | 7        | 0.23          |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG21 | 19       | 0.23          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 7        | 0.23          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 10       | 0.23          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 12       | 0.23          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 15       | 0.23          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 17       | 0.23          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 18       | 0.23          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 20       | 0.23          |
| (2,1677) | 2:1767:A:HIS:HB3  | 2:1781:A:ILE:HG21 | 6        | 0.23          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 19       | 0.23          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 16       | 0.23          |
| (2,1530) | 2:1746:A:ALA:HB3  | 2:1802:A:PRO:HB2  | 2        | 0.23          |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 16       | 0.23          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 18       | 0.23          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD11 | 14       | 0.23          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD11 | 15       | 0.23          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 17       | 0.23          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG22 | 12       | 0.23          |
| (2,1444) | 2:1796:A:CYS:HB2  | 2:1810:A:LYS:HE3  | 10       | 0.23          |
| (2,1414) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HB3   | 17       | 0.23          |
| (2,1397) | 2:1793:A:ALA:HB3  | 2:1794:A:LYS:H    | 9        | 0.23          |
| (2,1397) | 2:1793:A:ALA:HB1  | 2:1794:A:LYS:H    | 19       | 0.23          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG23 | 6        | 0.23          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 9        | 0.23          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 9        | 0.23          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 9        | 0.23          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 10       | 0.23          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 8        | 0.23          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 14       | 0.23          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 15       | 0.23          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 4        | 0.23          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 7        | 0.23          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 12       | 0.23          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 16       | 0.23          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG11 | 16       | 0.23          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 13       | 0.23          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 20       | 0.23          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 6        | 0.23          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 12       | 0.23          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 11       | 0.23          |
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 12       | 0.23          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 2        | 0.23          |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 13       | 0.23          |
| (2,1096) | 2:1737:A:ARG:HA   | 2:1737:A:ARG:HG3  | 17       | 0.23          |
| (2,1089) | 2:1774:A:LYS:HA   | 2:1779:A:CYS:HB2  | 18       | 0.23          |
| (2,1070) | 2:1782:A:CYS:HA   | 2:1768:A:THR:HG23 | 4        | 0.23          |
| (2,1069) | 2:1768:A:THR:HG21 | 2:1785:A:LEU:HD23 | 8        | 0.23          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 6        | 0.23          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 17       | 0.23          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 8        | 0.23          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 14       | 0.23          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 1        | 0.23          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 3        | 0.23          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 6        | 0.23          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 8        | 0.23          |
| (2,1038) | 2:1735:A:ILE:HG21 | 2:1736:A:GLN:H    | 14       | 0.23          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1038) | 2:1735:A:ILE:HG21 | 2:1736:A:GLN:H    | 16       | 0.23          |
| (2,1034) | 2:1735:A:ILE:HG21 | 2:1739:A:ILE:HB   | 2        | 0.23          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 1        | 0.23          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 19       | 0.23          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 20       | 0.23          |
| (2,1014) | 2:1733:A:LEU:HD23 | 2:1733:A:LEU:H    | 6        | 0.23          |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG23 | 6        | 0.23          |
| (2,951)  | 2:1780:A:PRO:HB3  | 1:134:B:ILE:HG21  | 16       | 0.23          |
| (2,857)  | 2:1750:A:ASN:HB2  | 2:1753:A:CYS:H    | 19       | 0.23          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 7        | 0.23          |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 2        | 0.23          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 1        | 0.23          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 5        | 0.23          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 8        | 0.23          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 8        | 0.23          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 10       | 0.23          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 20       | 0.23          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 15       | 0.23          |
| (2,754)  | 2:1774:A:LYS:HG2  | 2:1774:A:LYS:HE3  | 3        | 0.23          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 5        | 0.23          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 9        | 0.23          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 11       | 0.23          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 14       | 0.23          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 16       | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 5        | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 7        | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 10       | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 12       | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 13       | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 14       | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 15       | 0.23          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 20       | 0.23          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 4        | 0.23          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 19       | 0.23          |
| (2,636)  | 1:135:B:LEU:HD21  | 1:132:B:GLU:HB2   | 16       | 0.23          |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 17       | 0.23          |
| (2,558)  | 1:120:B:ILE:HD12  | 1:120:B:ILE:H     | 15       | 0.23          |
| (2,528)  | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 18       | 0.23          |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG22  | 9        | 0.23          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 5        | 0.23          |
| (2,470)  | 1:125:B:SER:H     | 1:124:B:ILE:HG23  | 16       | 0.23          |
| (2,464)  | 1:137:B:LEU:HD21  | 1:137:B:LEU:H     | 5        | 0.23          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,427)  | 1:136:B:GLY:H     | 1:135:B:LEU:HG    | 8        | 0.23          |
| (2,61)   | 2:1810:A:LYS:HG3  | 2:1810:A:LYS:H    | 5        | 0.23          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 4        | 0.23          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 8        | 0.23          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD3  | 6        | 0.22          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 12       | 0.22          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 11       | 0.22          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 13       | 0.22          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 14       | 0.22          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD1  | 16       | 0.22          |
| (2,1640) | 2:1807:A:LEU:HA   | 2:1810:A:LYS:HG3  | 9        | 0.22          |
| (2,1637) | 2:1810:A:LYS:HD2  | 2:1810:A:LYS:H    | 15       | 0.22          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 14       | 0.22          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 11       | 0.22          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 1        | 0.22          |
| (2,1530) | 2:1746:A:ALA:HB2  | 2:1802:A:PRO:HB2  | 18       | 0.22          |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 11       | 0.22          |
| (2,1506) | 2:1781:A:ILE:HD12 | 2:1781:A:ILE:H    | 14       | 0.22          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 3        | 0.22          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 13       | 0.22          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 15       | 0.22          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 17       | 0.22          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 19       | 0.22          |
| (2,1476) | 2:1805:A:PHE:HB3  | 2:1809:A:ILE:HD13 | 4        | 0.22          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD12 | 18       | 0.22          |
| (2,1466) | 2:1733:A:LEU:HA   | 2:1736:A:GLN:HG2  | 1        | 0.22          |
| (2,1457) | 2:1804:A:PRO:HD3  | 2:1803:A:VAL:HG23 | 13       | 0.22          |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 8        | 0.22          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 12       | 0.22          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 13       | 0.22          |
| (2,1376) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HA   | 1        | 0.22          |
| (2,1354) | 2:1780:A:PRO:HG2  | 2:1780:A:PRO:HD3  | 17       | 0.22          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 1        | 0.22          |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 9        | 0.22          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 10       | 0.22          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 13       | 0.22          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 20       | 0.22          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 5        | 0.22          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 13       | 0.22          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 3        | 0.22          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 18       | 0.22          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 20       | 0.22          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1155) | 2:1743:A:VAL:HG21 | 2:1744:A:HIS:H    | 13       | 0.22          |
| (2,1150) | 2:1743:A:VAL:HG23 | 2:1803:A:VAL:HG12 | 20       | 0.22          |
| (2,1146) | 2:1788:A:LEU:HD23 | 2:1735:A:ILE:HA   | 7        | 0.22          |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 10       | 0.22          |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 11       | 0.22          |
| (2,1127) | 2:1761:A:MET:HE2  | 2:1738:A:ALA:HB3  | 10       | 0.22          |
| (2,1127) | 2:1761:A:MET:HE2  | 2:1738:A:ALA:HB1  | 14       | 0.22          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 15       | 0.22          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 10       | 0.22          |
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 12       | 0.22          |
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 15       | 0.22          |
| (2,1034) | 2:1735:A:ILE:HG21 | 2:1739:A:ILE:HB   | 16       | 0.22          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 2        | 0.22          |
| (2,1014) | 2:1733:A:LEU:HD23 | 2:1733:A:LEU:H    | 2        | 0.22          |
| (2,1014) | 2:1733:A:LEU:HD21 | 2:1733:A:LEU:H    | 18       | 0.22          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG11 | 3        | 0.22          |
| (2,969)  | 2:1769:A:LYS:HD3  | 2:1766:A:GLN:HA   | 19       | 0.22          |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG23 | 19       | 0.22          |
| (2,929)  | 2:1768:A:THR:HB   | 2:1785:A:LEU:HD23 | 18       | 0.22          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 19       | 0.22          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 8        | 0.22          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 15       | 0.22          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 11       | 0.22          |
| (2,754)  | 2:1774:A:LYS:HG2  | 2:1774:A:LYS:HE3  | 10       | 0.22          |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 15       | 0.22          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE1  | 11       | 0.22          |
| (2,732)  | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HE2  | 19       | 0.22          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 2        | 0.22          |
| (2,657)  | 1:135:B:LEU:HD23  | 1:130:B:TYR:HD1   | 14       | 0.22          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 6        | 0.22          |
| (2,636)  | 1:135:B:LEU:HD21  | 1:132:B:GLU:HB2   | 1        | 0.22          |
| (2,576)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:H     | 11       | 0.22          |
| (2,576)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:H     | 19       | 0.22          |
| (2,540)  | 1:134:B:ILE:HG21  | 2:1781:A:ILE:HA   | 18       | 0.22          |
| (2,470)  | 1:125:B:SER:H     | 1:124:B:ILE:HG23  | 5        | 0.22          |
| (2,467)  | 1:124:B:ILE:HG22  | 1:124:B:ILE:HG12  | 16       | 0.22          |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 14       | 0.22          |
| (2,247)  | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 7        | 0.22          |
| (2,170)  | 2:1750:A:ASN:H    | 2:1749:A:ARG:HB2  | 17       | 0.22          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 10       | 0.22          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 20       | 0.22          |
| (2,22)   | 2:1809:A:ILE:HG21 | 2:1809:A:ILE:H    | 6        | 0.22          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 14       | 0.22          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 9        | 0.22          |
| (3,36)   | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG3  | 17       | 0.21          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG21 | 10       | 0.21          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG23 | 2        | 0.21          |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG22 | 5        | 0.21          |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG23 | 13       | 0.21          |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 5        | 0.21          |
| (2,1699) | 2:1781:A:ILE:HD12 | 2:1767:A:HIS:HD2  | 8        | 0.21          |
| (2,1698) | 2:1788:A:LEU:HD21 | 2:1787:A:ALA:H    | 18       | 0.21          |
| (2,1680) | 2:1797:A:GLN:HG2  | 2:1796:A:CYS:HA   | 17       | 0.21          |
| (2,1677) | 2:1767:A:HIS:HB3  | 2:1781:A:ILE:HG23 | 18       | 0.21          |
| (2,1635) | 2:1788:A:LEU:HD13 | 1:130:B:TYR:HE1   | 7        | 0.21          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 9        | 0.21          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB2  | 20       | 0.21          |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE1   | 8        | 0.21          |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE2   | 9        | 0.21          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 6        | 0.21          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 2        | 0.21          |
| (2,1506) | 2:1781:A:ILE:HD11 | 2:1781:A:ILE:H    | 12       | 0.21          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 11       | 0.21          |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD12 | 2        | 0.21          |
| (2,1379) | 2:1809:A:ILE:HG23 | 2:1793:A:ALA:HB3  | 14       | 0.21          |
| (2,1377) | 2:1809:A:ILE:HA   | 2:1809:A:ILE:HG21 | 9        | 0.21          |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 2        | 0.21          |
| (2,1376) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HA   | 3        | 0.21          |
| (2,1376) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HA   | 5        | 0.21          |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 17       | 0.21          |
| (2,1371) | 2:1764:A:VAL:HG21 | 2:1764:A:VAL:H    | 10       | 0.21          |
| (2,1358) | 2:1742:A:LEU:HD12 | 2:1803:A:VAL:HG13 | 8        | 0.21          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 19       | 0.21          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 20       | 0.21          |
| (2,1343) | 2:1755:A:LEU:HD21 | 2:1755:A:LEU:HA   | 17       | 0.21          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 5        | 0.21          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 6        | 0.21          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 15       | 0.21          |
| (2,1281) | 2:1736:A:GLN:HG2  | 2:1736:A:GLN:H    | 11       | 0.21          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 5        | 0.21          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 8        | 0.21          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 16       | 0.21          |
| (2,1241) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:HE2  | 19       | 0.21          |
| (2,1212) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:H    | 7        | 0.21          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1201) | 2:1801:A:CYS:HA   | 2:1802:A:PRO:HG2  | 20       | 0.21          |
| (2,1193) | 2:1775:A:THR:HA   | 2:1774:A:LYS:HG3  | 18       | 0.21          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 8        | 0.21          |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 10       | 0.21          |
| (2,1175) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:HA   | 12       | 0.21          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 18       | 0.21          |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 13       | 0.21          |
| (2,1133) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:HG2  | 12       | 0.21          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 7        | 0.21          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 15       | 0.21          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 4        | 0.21          |
| (2,1038) | 2:1735:A:ILE:HG21 | 2:1736:A:GLN:H    | 5        | 0.21          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 13       | 0.21          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 17       | 0.21          |
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 18       | 0.21          |
| (2,1038) | 2:1735:A:ILE:HG23 | 2:1736:A:GLN:H    | 19       | 0.21          |
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 20       | 0.21          |
| (2,1035) | 2:1739:A:ILE:HG12 | 2:1735:A:ILE:HG23 | 16       | 0.21          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 8        | 0.21          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 15       | 0.21          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 17       | 0.21          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 18       | 0.21          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 17       | 0.21          |
| (2,987)  | 2:1764:A:VAL:HA   | 2:1781:A:ILE:HG23 | 20       | 0.21          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 14       | 0.21          |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 4        | 0.21          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD13 | 15       | 0.21          |
| (2,878)  | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 3        | 0.21          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 17       | 0.21          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 1        | 0.21          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 20       | 0.21          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 13       | 0.21          |
| (2,786)  | 2:1805:A:PHE:HB2  | 2:1809:A:ILE:HD13 | 3        | 0.21          |
| (2,786)  | 2:1805:A:PHE:HB2  | 2:1809:A:ILE:HD13 | 16       | 0.21          |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 1        | 0.21          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 1        | 0.21          |
| (2,731)  | 2:1791:A:TYR:HB2  | 2:1792:A:HIS:H    | 7        | 0.21          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 1        | 0.21          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 13       | 0.21          |
| (2,671)  | 1:126:B:LEU:HG    | 1:122:B:ASP:HB2   | 19       | 0.21          |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE2   | 15       | 0.21          |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 11       | 0.21          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 20       | 0.21          |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG21  | 4        | 0.21          |
| (2,576)  | 1:119:B:VAL:HG11  | 1:120:B:ILE:H     | 6        | 0.21          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 6        | 0.21          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 13       | 0.21          |
| (2,524)  | 1:137:B:LEU:HD12  | 1:137:B:LEU:HB2   | 5        | 0.21          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG22  | 2        | 0.21          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 12       | 0.21          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 15       | 0.21          |
| (2,261)  | 2:1747:A:GLN:H    | 2:1745:A:ALA:HB1  | 4        | 0.21          |
| (2,238)  | 2:1779:A:CYS:H    | 2:1773:A:ARG:HD3  | 18       | 0.21          |
| (2,210)  | 2:1739:A:ILE:HG23 | 2:1739:A:ILE:H    | 9        | 0.21          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 11       | 0.21          |
| (2,114)  | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 17       | 0.21          |
| (2,22)   | 2:1809:A:ILE:HG23 | 2:1809:A:ILE:H    | 8        | 0.21          |
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 9        | 0.21          |
| (2,1)    | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD21 | 17       | 0.21          |
| (3,36)   | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG3  | 3        | 0.2           |
| (3,36)   | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG3  | 7        | 0.2           |
| (3,12)   | 1:123:B:ILE:HA    | 1:126:B:LEU:HD22  | 1        | 0.2           |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 2        | 0.2           |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 7        | 0.2           |
| (2,1739) | 2:1792:A:HIS:HA   | 2:1791:A:TYR:HD2  | 16       | 0.2           |
| (2,1737) | 2:1785:A:LEU:HD11 | 2:1767:A:HIS:HD2  | 1        | 0.2           |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 11       | 0.2           |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG22 | 3        | 0.2           |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG22 | 7        | 0.2           |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG23 | 11       | 0.2           |
| (2,1715) | 2:1791:A:TYR:HB2  | 2:1791:A:TYR:HD2  | 19       | 0.2           |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 14       | 0.2           |
| (2,1664) | 2:1811:A:GLN:HG3  | 2:1811:A:GLN:H    | 3        | 0.2           |
| (2,1664) | 2:1811:A:GLN:HG3  | 2:1811:A:GLN:H    | 8        | 0.2           |
| (2,1637) | 2:1810:A:LYS:HD2  | 2:1810:A:LYS:H    | 16       | 0.2           |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB1  | 19       | 0.2           |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 5        | 0.2           |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 18       | 0.2           |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 1        | 0.2           |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 19       | 0.2           |
| (2,1572) | 2:1809:A:ILE:HD13 | 2:1805:A:PHE:HD2  | 13       | 0.2           |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 5        | 0.2           |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 12       | 0.2           |
| (2,1530) | 2:1746:A:ALA:HB2  | 2:1802:A:PRO:HB2  | 6        | 0.2           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 5        | 0.2           |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 20       | 0.2           |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD12 | 5        | 0.2           |
| (2,1451) | 2:1789:A:ALA:HB1  | 2:1805:A:PHE:HD2  | 5        | 0.2           |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 3        | 0.2           |
| (2,1428) | 2:1790:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 9        | 0.2           |
| (2,1397) | 2:1793:A:ALA:HB1  | 2:1794:A:LYS:H    | 7        | 0.2           |
| (2,1397) | 2:1793:A:ALA:HB3  | 2:1794:A:LYS:H    | 14       | 0.2           |
| (2,1387) | 2:1785:A:LEU:HD12 | 2:1805:A:PHE:HE2  | 15       | 0.2           |
| (2,1379) | 2:1809:A:ILE:HG22 | 2:1793:A:ALA:HB1  | 19       | 0.2           |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 4        | 0.2           |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 14       | 0.2           |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 15       | 0.2           |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 3        | 0.2           |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 6        | 0.2           |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 18       | 0.2           |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 5        | 0.2           |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 7        | 0.2           |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 9        | 0.2           |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 19       | 0.2           |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 4        | 0.2           |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 8        | 0.2           |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 16       | 0.2           |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 19       | 0.2           |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG12 | 9        | 0.2           |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG13 | 20       | 0.2           |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 20       | 0.2           |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 9        | 0.2           |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 10       | 0.2           |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 18       | 0.2           |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 19       | 0.2           |
| (2,1219) | 2:1800:A:LYS:HG3  | 2:1800:A:LYS:HE2  | 13       | 0.2           |
| (2,1193) | 2:1775:A:THR:HA   | 2:1774:A:LYS:HG3  | 8        | 0.2           |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 3        | 0.2           |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 16       | 0.2           |
| (2,1175) | 2:1755:A:LEU:HD11 | 2:1755:A:LEU:HA   | 1        | 0.2           |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 4        | 0.2           |
| (2,1175) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:HA   | 6        | 0.2           |
| (2,1175) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:HA   | 14       | 0.2           |
| (2,1175) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:HA   | 17       | 0.2           |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 1        | 0.2           |
| (2,1155) | 2:1743:A:VAL:HG21 | 2:1744:A:HIS:H    | 16       | 0.2           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1146) | 2:1788:A:LEU:HD21 | 2:1735:A:ILE:HA   | 3        | 0.2           |
| (2,1135) | 2:1765:A:VAL:HG11 | 2:1804:A:PRO:HG2  | 19       | 0.2           |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 16       | 0.2           |
| (2,1072) | 2:1768:A:THR:HG21 | 2:1805:A:PHE:HE1  | 5        | 0.2           |
| (2,1069) | 2:1768:A:THR:HG23 | 2:1785:A:LEU:HD22 | 13       | 0.2           |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 19       | 0.2           |
| (2,1038) | 2:1735:A:ILE:HG21 | 2:1736:A:GLN:H    | 2        | 0.2           |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 6        | 0.2           |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 14       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 1        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 2        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 3        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 4        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 5        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 6        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 7        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 8        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 9        | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 10       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 11       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 12       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 13       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 14       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 15       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 16       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 17       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 18       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 19       | 0.2           |
| (2,972)  | 2:1788:A:LEU:HA   | 2:1788:A:LEU:HB2  | 20       | 0.2           |
| (2,971)  | 2:1734:A:SER:HB3  | 2:1733:A:LEU:HD11 | 6        | 0.2           |
| (2,954)  | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 9        | 0.2           |
| (2,923)  | 2:1765:A:VAL:HG21 | 2:1745:A:ALA:HB1  | 5        | 0.2           |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB2  | 17       | 0.2           |
| (2,881)  | 2:1807:A:LEU:HG   | 2:1801:A:CYS:HB2  | 11       | 0.2           |
| (2,845)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HD3  | 2        | 0.2           |
| (2,836)  | 2:1771:A:CYS:HB3  | 2:1771:A:CYS:H    | 12       | 0.2           |
| (2,826)  | 2:1791:A:TYR:HA   | 2:1794:A:LYS:HB2  | 11       | 0.2           |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 12       | 0.2           |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 17       | 0.2           |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 14       | 0.2           |
| (2,756)  | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:H    | 10       | 0.2           |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 2        | 0.2           |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 6        | 0.2           |
| (2,743)  | 2:1769:A:LYS:HG3  | 2:1769:A:LYS:H    | 8        | 0.2           |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 19       | 0.2           |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 3        | 0.2           |
| (2,636)  | 1:135:B:LEU:HD21  | 1:132:B:GLU:HB2   | 7        | 0.2           |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG21  | 10       | 0.2           |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 6        | 0.2           |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 15       | 0.2           |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 20       | 0.2           |
| (2,467)  | 1:124:B:ILE:HG22  | 1:124:B:ILE:HG12  | 5        | 0.2           |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 20       | 0.2           |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 9        | 0.2           |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 2        | 0.2           |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 5        | 0.2           |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 19       | 0.2           |
| (2,114)  | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 2        | 0.2           |
| (2,22)   | 2:1809:A:ILE:HG23 | 2:1809:A:ILE:H    | 3        | 0.2           |
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 4        | 0.2           |
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 10       | 0.2           |
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 13       | 0.2           |
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 18       | 0.2           |
| (1,35)   | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 14       | 0.2           |
| (3,36)   | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG3  | 13       | 0.19          |
| (3,20)   | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HD2  | 5        | 0.19          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 2        | 0.19          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 8        | 0.19          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 12       | 0.19          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG23 | 16       | 0.19          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 20       | 0.19          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 17       | 0.19          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG21 | 9        | 0.19          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG23 | 12       | 0.19          |
| (2,1716) | 2:1785:A:LEU:HB2  | 2:1805:A:PHE:HE1  | 8        | 0.19          |
| (2,1699) | 2:1781:A:ILE:HD12 | 2:1767:A:HIS:HD2  | 17       | 0.19          |
| (2,1698) | 2:1788:A:LEU:HD23 | 2:1787:A:ALA:H    | 3        | 0.19          |
| (2,1637) | 2:1810:A:LYS:HD2  | 2:1810:A:LYS:H    | 1        | 0.19          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB1  | 6        | 0.19          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB2  | 12       | 0.19          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 4        | 0.19          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 11       | 0.19          |
| (2,1572) | 2:1809:A:ILE:HD11 | 2:1805:A:PHE:HD1  | 18       | 0.19          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 3        | 0.19          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 4        | 0.19          |
| (2,1530) | 2:1746:A:ALA:HB3  | 2:1802:A:PRO:HB2  | 4        | 0.19          |
| (2,1515) | 2:1764:A:VAL:HG11 | 2:1761:A:MET:HG2  | 10       | 0.19          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 2        | 0.19          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 7        | 0.19          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 14       | 0.19          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD13 | 20       | 0.19          |
| (2,1451) | 2:1789:A:ALA:HB1  | 2:1805:A:PHE:HD2  | 7        | 0.19          |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 1        | 0.19          |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 11       | 0.19          |
| (2,1414) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HB3   | 3        | 0.19          |
| (2,1414) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HB3   | 4        | 0.19          |
| (2,1376) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HA   | 7        | 0.19          |
| (2,1376) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HA   | 8        | 0.19          |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 10       | 0.19          |
| (2,1376) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HA   | 16       | 0.19          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 16       | 0.19          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 5        | 0.19          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 8        | 0.19          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 12       | 0.19          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 11       | 0.19          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 12       | 0.19          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 13       | 0.19          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 16       | 0.19          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 18       | 0.19          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 19       | 0.19          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 19       | 0.19          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 2        | 0.19          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 12       | 0.19          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 14       | 0.19          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 11       | 0.19          |
| (2,1219) | 2:1800:A:LYS:HG3  | 2:1800:A:LYS:HE2  | 1        | 0.19          |
| (2,1176) | 2:1755:A:LEU:HD11 | 2:1756:A:PRO:HD3  | 15       | 0.19          |
| (2,1176) | 2:1755:A:LEU:HD13 | 2:1756:A:PRO:HD3  | 20       | 0.19          |
| (2,1157) | 2:1743:A:VAL:HG21 | 2:1747:A:GLN:HE21 | 16       | 0.19          |
| (2,1155) | 2:1743:A:VAL:HG23 | 2:1744:A:HIS:H    | 6        | 0.19          |
| (2,1146) | 2:1788:A:LEU:HD23 | 2:1735:A:ILE:HA   | 1        | 0.19          |
| (2,1135) | 2:1765:A:VAL:HG12 | 2:1804:A:PRO:HG2  | 5        | 0.19          |
| (2,1119) | 2:1739:A:ILE:HG23 | 2:1736:A:GLN:HA   | 4        | 0.19          |
| (2,1105) | 2:1774:A:LYS:HE3  | 2:1805:A:PHE:HE2  | 14       | 0.19          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 4        | 0.19          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 19       | 0.19          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 4        | 0.19          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 13       | 0.19          |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 14       | 0.19          |
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 11       | 0.19          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 7        | 0.19          |
| (2,998)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HG3  | 6        | 0.19          |
| (2,986)  | 2:1764:A:VAL:HA   | 2:1764:A:VAL:HG12 | 2        | 0.19          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD12 | 8        | 0.19          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 9        | 0.19          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 16       | 0.19          |
| (2,924)  | 2:1765:A:VAL:HG21 | 2:1746:A:ALA:HB1  | 5        | 0.19          |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB3  | 1        | 0.19          |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB3  | 7        | 0.19          |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB1  | 18       | 0.19          |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 1        | 0.19          |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 2        | 0.19          |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 4        | 0.19          |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 12       | 0.19          |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 15       | 0.19          |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 16       | 0.19          |
| (2,891)  | 2:1800:A:LYS:HB2  | 2:1800:A:LYS:HA   | 17       | 0.19          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 19       | 0.19          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 11       | 0.19          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 13       | 0.19          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 16       | 0.19          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 14       | 0.19          |
| (2,757)  | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H    | 19       | 0.19          |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 20       | 0.19          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 5        | 0.19          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 15       | 0.19          |
| (2,685)  | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG2  | 7        | 0.19          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD2   | 15       | 0.19          |
| (2,645)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1   | 6        | 0.19          |
| (2,638)  | 1:115:B:GLN:HG2   | 1:115:B:GLN:HA    | 19       | 0.19          |
| (2,593)  | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG23  | 5        | 0.19          |
| (2,576)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:H     | 5        | 0.19          |
| (2,576)  | 1:119:B:VAL:HG13  | 1:120:B:ILE:H     | 16       | 0.19          |
| (2,555)  | 1:124:B:ILE:HD11  | 1:124:B:ILE:HB    | 16       | 0.19          |
| (2,522)  | 1:135:B:LEU:HD13  | 1:135:B:LEU:HA    | 2        | 0.19          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG23  | 5        | 0.19          |
| (2,519)  | 1:125:B:SER:HB2   | 1:124:B:ILE:HG23  | 15       | 0.19          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 1        | 0.19          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 8        | 0.19          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 9        | 0.19          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 17       | 0.19          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD2   | 13       | 0.19          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG21  | 3        | 0.19          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 13       | 0.19          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG22  | 17       | 0.19          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG21  | 19       | 0.19          |
| (2,470)  | 1:125:B:SER:H     | 1:124:B:ILE:HG22  | 6        | 0.19          |
| (2,469)  | 1:126:B:LEU:HD23  | 2:1787:A:ALA:HA   | 9        | 0.19          |
| (2,467)  | 1:124:B:ILE:HG21  | 1:124:B:ILE:HG12  | 6        | 0.19          |
| (2,386)  | 1:126:B:LEU:H     | 1:126:B:LEU:HD11  | 9        | 0.19          |
| (2,321)  | 2:1777:A:GLY:H    | 2:1776:A:ASN:HA   | 10       | 0.19          |
| (2,238)  | 2:1779:A:CYS:H    | 2:1773:A:ARG:HD3  | 14       | 0.19          |
| (2,175)  | 2:1773:A:ARG:H    | 2:1772:A:LYS:HB2  | 20       | 0.19          |
| (2,37)   | 2:1766:A:GLN:HE22 | 2:1766:A:GLN:HG2  | 17       | 0.19          |
| (2,22)   | 2:1809:A:ILE:HG21 | 2:1809:A:ILE:H    | 1        | 0.19          |
| (2,22)   | 2:1809:A:ILE:HG21 | 2:1809:A:ILE:H    | 19       | 0.19          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 6        | 0.18          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG23 | 11       | 0.18          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG23 | 20       | 0.18          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 15       | 0.18          |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 18       | 0.18          |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 19       | 0.18          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 3        | 0.18          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 19       | 0.18          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG21 | 1        | 0.18          |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG23 | 10       | 0.18          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG22 | 15       | 0.18          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG23 | 20       | 0.18          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 8        | 0.18          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 17       | 0.18          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 18       | 0.18          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 16       | 0.18          |
| (2,1570) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HE1   | 4        | 0.18          |
| (2,1570) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HE2   | 17       | 0.18          |
| (2,1555) | 2:1735:A:ILE:HD12 | 1:130:B:TYR:HD1   | 15       | 0.18          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 6        | 0.18          |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 17       | 0.18          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 4        | 0.18          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 6        | 0.18          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 16       | 0.18          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 19       | 0.18          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD11 | 11       | 0.18          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD13 | 17       | 0.18          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 6        | 0.18          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 10       | 0.18          |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 18       | 0.18          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 1        | 0.18          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 20       | 0.18          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 7        | 0.18          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 18       | 0.18          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 1        | 0.18          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 7        | 0.18          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 2        | 0.18          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 6        | 0.18          |
| (2,1349) | 2:1783:A:LYS:HG2  | 2:1783:A:LYS:HB2  | 20       | 0.18          |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 6        | 0.18          |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 10       | 0.18          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 12       | 0.18          |
| (2,1343) | 2:1755:A:LEU:HD22 | 2:1755:A:LEU:HA   | 14       | 0.18          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 18       | 0.18          |
| (2,1263) | 2:1772:A:LYS:HE3  | 2:1772:A:LYS:HB2  | 18       | 0.18          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 4        | 0.18          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 7        | 0.18          |
| (2,1253) | 2:1727:A:PRO:HA   | 2:1727:A:PRO:HB2  | 11       | 0.18          |
| (2,1219) | 2:1800:A:LYS:HG3  | 2:1800:A:LYS:HE2  | 18       | 0.18          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 2        | 0.18          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 5        | 0.18          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 7        | 0.18          |
| (2,1176) | 2:1755:A:LEU:HD11 | 2:1756:A:PRO:HD3  | 9        | 0.18          |
| (2,1176) | 2:1755:A:LEU:HD11 | 2:1756:A:PRO:HD3  | 11       | 0.18          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 19       | 0.18          |
| (2,1158) | 2:1758:A:CYS:HA   | 2:1761:A:MET:HB2  | 11       | 0.18          |
| (2,1158) | 2:1758:A:CYS:HA   | 2:1761:A:MET:HB2  | 20       | 0.18          |
| (2,1146) | 2:1788:A:LEU:HD22 | 2:1735:A:ILE:HA   | 18       | 0.18          |
| (2,1136) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:H    | 6        | 0.18          |
| (2,1133) | 2:1765:A:VAL:HG12 | 2:1766:A:GLN:HG2  | 3        | 0.18          |
| (2,1127) | 2:1761:A:MET:HE1  | 2:1738:A:ALA:HB3  | 7        | 0.18          |
| (2,1119) | 2:1739:A:ILE:HG23 | 2:1736:A:GLN:HA   | 12       | 0.18          |
| (2,1103) | 2:1774:A:LYS:HE3  | 2:1774:A:LYS:HD3  | 18       | 0.18          |
| (2,1083) | 2:1781:A:ILE:HG21 | 2:1785:A:LEU:HD23 | 17       | 0.18          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 2        | 0.18          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 9        | 0.18          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1038) | 2:1735:A:ILE:HG22 | 2:1736:A:GLN:H    | 7        | 0.18          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 4        | 0.18          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 6        | 0.18          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 11       | 0.18          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 16       | 0.18          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 1        | 0.18          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 2        | 0.18          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 9        | 0.18          |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG21 | 12       | 0.18          |
| (2,923)  | 2:1765:A:VAL:HG22 | 2:1745:A:ALA:HB3  | 10       | 0.18          |
| (2,906)  | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA   | 9        | 0.18          |
| (2,906)  | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA   | 10       | 0.18          |
| (2,881)  | 2:1807:A:LEU:HG   | 2:1801:A:CYS:HB2  | 12       | 0.18          |
| (2,835)  | 2:1771:A:CYS:HB3  | 2:1768:A:THR:HA   | 4        | 0.18          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 2        | 0.18          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 6        | 0.18          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 15       | 0.18          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 5        | 0.18          |
| (2,681)  | 1:139:B:ASP:HB2   | 1:140:B:PRO:HD2   | 11       | 0.18          |
| (2,669)  | 1:120:B:ILE:HG21  | 1:117:B:ASP:H     | 12       | 0.18          |
| (2,657)  | 1:135:B:LEU:HD23  | 1:130:B:TYR:HD1   | 20       | 0.18          |
| (2,646)  | 1:132:B:GLU:HB2   | 1:130:B:TYR:HD2   | 3        | 0.18          |
| (2,636)  | 1:135:B:LEU:HD23  | 1:132:B:GLU:HB2   | 8        | 0.18          |
| (2,569)  | 1:124:B:ILE:HA    | 1:124:B:ILE:HG22  | 15       | 0.18          |
| (2,540)  | 1:134:B:ILE:HG22  | 2:1781:A:ILE:HA   | 5        | 0.18          |
| (2,522)  | 1:135:B:LEU:HD11  | 1:135:B:LEU:HA    | 4        | 0.18          |
| (2,522)  | 1:135:B:LEU:HD12  | 1:135:B:LEU:HA    | 12       | 0.18          |
| (2,510)  | 1:117:B:ASP:HA    | 1:119:B:VAL:HG22  | 9        | 0.18          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 4        | 0.18          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 9        | 0.18          |
| (2,475)  | 1:130:B:TYR:HA    | 1:130:B:TYR:HD1   | 19       | 0.18          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 1        | 0.18          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG21  | 6        | 0.18          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 8        | 0.18          |
| (2,431)  | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 9        | 0.18          |
| (2,356)  | 1:121:B:ASP:H     | 1:121:B:ASP:HB3   | 3        | 0.18          |
| (2,247)  | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 9        | 0.18          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 15       | 0.18          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 12       | 0.18          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 13       | 0.18          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 15       | 0.18          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 16       | 0.18          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 17       | 0.18          |
| (2,108)  | 2:1741:A:SER:H    | 2:1761:A:MET:HE1  | 12       | 0.18          |
| (2,108)  | 2:1741:A:SER:H    | 2:1761:A:MET:HE3  | 20       | 0.18          |
| (2,37)   | 2:1766:A:GLN:HE22 | 2:1766:A:GLN:HG2  | 3        | 0.18          |
| (2,22)   | 2:1809:A:ILE:HG23 | 2:1809:A:ILE:H    | 5        | 0.18          |
| (2,22)   | 2:1809:A:ILE:HG21 | 2:1809:A:ILE:H    | 7        | 0.18          |
| (2,22)   | 2:1809:A:ILE:HG23 | 2:1809:A:ILE:H    | 12       | 0.18          |
| (2,22)   | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 15       | 0.18          |
| (3,36)   | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG3  | 8        | 0.17          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 4        | 0.17          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG21 | 7        | 0.17          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 17       | 0.17          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 18       | 0.17          |
| (3,9)    | 1:120:B:ILE:HG23  | 1:120:B:ILE:HG12  | 17       | 0.17          |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 10       | 0.17          |
| (2,1737) | 2:1785:A:LEU:HD13 | 2:1767:A:HIS:HD2  | 16       | 0.17          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 12       | 0.17          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 4        | 0.17          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 15       | 0.17          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 17       | 0.17          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG21 | 6        | 0.17          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG22 | 16       | 0.17          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG22 | 17       | 0.17          |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG21 | 18       | 0.17          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 5        | 0.17          |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE2  | 20       | 0.17          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 3        | 0.17          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 12       | 0.17          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 13       | 0.17          |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 3        | 0.17          |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE1   | 1        | 0.17          |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE1   | 7        | 0.17          |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE2   | 16       | 0.17          |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 7        | 0.17          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 11       | 0.17          |
| (2,1514) | 2:1764:A:VAL:HG12 | 2:1781:A:ILE:HG22 | 10       | 0.17          |
| (2,1506) | 2:1781:A:ILE:HD12 | 2:1781:A:ILE:H    | 10       | 0.17          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 8        | 0.17          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 12       | 0.17          |
| (2,1428) | 2:1790:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 4        | 0.17          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 5        | 0.17          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 17       | 0.17          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1397) | 2:1793:A:ALA:HB1  | 2:1794:A:LYS:H    | 2        | 0.17          |
| (2,1376) | 2:1809:A:ILE:HG23 | 2:1810:A:LYS:HA   | 12       | 0.17          |
| (2,1376) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HA   | 19       | 0.17          |
| (2,1376) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HA   | 20       | 0.17          |
| (2,1371) | 2:1764:A:VAL:HG22 | 2:1764:A:VAL:H    | 7        | 0.17          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 10       | 0.17          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 5        | 0.17          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 15       | 0.17          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 11       | 0.17          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 16       | 0.17          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 19       | 0.17          |
| (2,1343) | 2:1755:A:LEU:HD23 | 2:1755:A:LEU:HA   | 8        | 0.17          |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 3        | 0.17          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 2        | 0.17          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 14       | 0.17          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG12 | 18       | 0.17          |
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 20       | 0.17          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 3        | 0.17          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 17       | 0.17          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 13       | 0.17          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 18       | 0.17          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 3        | 0.17          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 7        | 0.17          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 13       | 0.17          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 15       | 0.17          |
| (2,1153) | 2:1743:A:VAL:HG23 | 2:1747:A:GLN:HG2  | 16       | 0.17          |
| (2,1150) | 2:1743:A:VAL:HG22 | 2:1803:A:VAL:HG13 | 17       | 0.17          |
| (2,1079) | 2:1782:A:CYS:HA   | 2:1781:A:ILE:HG21 | 9        | 0.17          |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 1        | 0.17          |
| (2,1054) | 2:1783:A:LYS:HD3  | 2:1780:A:PRO:HA   | 8        | 0.17          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 10       | 0.17          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 20       | 0.17          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 3        | 0.17          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 7        | 0.17          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 10       | 0.17          |
| (2,1006) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HB3  | 7        | 0.17          |
| (2,969)  | 2:1769:A:LYS:HD3  | 2:1766:A:GLN:HA   | 18       | 0.17          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD13 | 1        | 0.17          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD13 | 10       | 0.17          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 15       | 0.17          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 16       | 0.17          |
| (2,960)  | 2:1739:A:ILE:HD11 | 2:1735:A:ILE:HG22 | 13       | 0.17          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (2,957) | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 2        | 0.17          |
| (2,957) | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 11       | 0.17          |
| (2,957) | 2:1763:A:ARG:HD2  | 2:1763:A:ARG:HG2  | 14       | 0.17          |
| (2,953) | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 3        | 0.17          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 11       | 0.17          |
| (2,913) | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 12       | 0.17          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 8        | 0.17          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1  | 20       | 0.17          |
| (2,806) | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 4        | 0.17          |
| (2,806) | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 9        | 0.17          |
| (2,786) | 2:1805:A:PHE:HB2  | 2:1809:A:ILE:HD12 | 4        | 0.17          |
| (2,749) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 14       | 0.17          |
| (2,742) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 10       | 0.17          |
| (2,723) | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 6        | 0.17          |
| (2,723) | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 18       | 0.17          |
| (2,543) | 1:134:B:ILE:HG12  | 1:134:B:ILE:HA    | 15       | 0.17          |
| (2,528) | 1:133:B:GLU:HG3   | 1:134:B:ILE:H     | 10       | 0.17          |
| (2,522) | 1:135:B:LEU:HD12  | 1:135:B:LEU:HA    | 7        | 0.17          |
| (2,522) | 1:135:B:LEU:HD13  | 1:135:B:LEU:HA    | 9        | 0.17          |
| (2,513) | 1:126:B:LEU:HD11  | 1:123:B:ILE:HA    | 18       | 0.17          |
| (2,500) | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 20       | 0.17          |
| (2,455) | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 4        | 0.17          |
| (2,455) | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 5        | 0.17          |
| (2,427) | 1:136:B:GLY:H     | 1:135:B:LEU:HG    | 10       | 0.17          |
| (2,356) | 1:121:B:ASP:H     | 1:121:B:ASP:HB3   | 16       | 0.17          |
| (2,338) | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 11       | 0.17          |
| (2,321) | 2:1777:A:GLY:H    | 2:1776:A:ASN:HA   | 16       | 0.17          |
| (2,247) | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 15       | 0.17          |
| (2,114) | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 1        | 0.17          |
| (2,114) | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 8        | 0.17          |
| (2,114) | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 10       | 0.17          |
| (2,114) | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 12       | 0.17          |
| (2,37)  | 2:1766:A:GLN:HE22 | 2:1766:A:GLN:HG2  | 7        | 0.17          |
| (2,37)  | 2:1766:A:GLN:HE22 | 2:1766:A:GLN:HG2  | 10       | 0.17          |
| (2,22)  | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 2        | 0.17          |
| (2,22)  | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 11       | 0.17          |
| (2,22)  | 2:1809:A:ILE:HG21 | 2:1809:A:ILE:H    | 16       | 0.17          |
| (2,22)  | 2:1809:A:ILE:HG22 | 2:1809:A:ILE:H    | 17       | 0.17          |
| (2,1)   | 2:1785:A:LEU:H    | 2:1785:A:LEU:HD22 | 10       | 0.17          |
| (1,35)  | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 1        | 0.17          |
| (1,35)  | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 12       | 0.17          |
| (1,35)  | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 13       | 0.17          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (3,36)   | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG3  | 10       | 0.16          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 2        | 0.16          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG23 | 1        | 0.16          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 5        | 0.16          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 9        | 0.16          |
| (3,9)    | 1:120:B:ILE:HG23  | 1:120:B:ILE:HG12  | 10       | 0.16          |
| (3,9)    | 1:120:B:ILE:HG23  | 1:120:B:ILE:HG12  | 13       | 0.16          |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 5        | 0.16          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 12       | 0.16          |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 13       | 0.16          |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 14       | 0.16          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 4        | 0.16          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 5        | 0.16          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 7        | 0.16          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 8        | 0.16          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 10       | 0.16          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 18       | 0.16          |
| (2,1727) | 2:1781:A:ILE:HG21 | 2:1767:A:HIS:HD2  | 14       | 0.16          |
| (2,1721) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HG22 | 14       | 0.16          |
| (2,1637) | 2:1810:A:LYS:HD2  | 2:1810:A:LYS:H    | 13       | 0.16          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 8        | 0.16          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 15       | 0.16          |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 12       | 0.16          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 1        | 0.16          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 4        | 0.16          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 6        | 0.16          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 12       | 0.16          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 14       | 0.16          |
| (2,1570) | 2:1788:A:LEU:HD22 | 1:130:B:TYR:HE2   | 18       | 0.16          |
| (2,1551) | 2:1735:A:ILE:HG21 | 2:1791:A:TYR:HB2  | 1        | 0.16          |
| (2,1551) | 2:1735:A:ILE:HG22 | 2:1791:A:TYR:HB2  | 16       | 0.16          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 13       | 0.16          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 15       | 0.16          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 17       | 0.16          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 20       | 0.16          |
| (2,1530) | 2:1746:A:ALA:HB3  | 2:1802:A:PRO:HB2  | 5        | 0.16          |
| (2,1530) | 2:1746:A:ALA:HB3  | 2:1802:A:PRO:HB2  | 8        | 0.16          |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 10       | 0.16          |
| (2,1530) | 2:1746:A:ALA:HB3  | 2:1802:A:PRO:HB2  | 11       | 0.16          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 9        | 0.16          |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 12       | 0.16          |
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 3        | 0.16          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1515) | 2:1764:A:VAL:HG13 | 2:1761:A:MET:HG2  | 20       | 0.16          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 17       | 0.16          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD13 | 8        | 0.16          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD13 | 12       | 0.16          |
| (2,1471) | 2:1798:A:GLU:HA   | 2:1798:A:GLU:HG2  | 15       | 0.16          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD11 | 15       | 0.16          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 18       | 0.16          |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD13 | 20       | 0.16          |
| (2,1397) | 2:1793:A:ALA:HB3  | 2:1794:A:LYS:H    | 3        | 0.16          |
| (2,1383) | 2:1785:A:LEU:HD11 | 2:1785:A:LEU:HA   | 5        | 0.16          |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 11       | 0.16          |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 18       | 0.16          |
| (2,1371) | 2:1764:A:VAL:HG21 | 2:1764:A:VAL:H    | 13       | 0.16          |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 10       | 0.16          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 1        | 0.16          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 17       | 0.16          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB2  | 7        | 0.16          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG11 | 19       | 0.16          |
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 13       | 0.16          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 15       | 0.16          |
| (2,1259) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HB2  | 6        | 0.16          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 3        | 0.16          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 9        | 0.16          |
| (2,1219) | 2:1800:A:LYS:HG3  | 2:1800:A:LYS:HE2  | 12       | 0.16          |
| (2,1219) | 2:1800:A:LYS:HG3  | 2:1800:A:LYS:HE2  | 14       | 0.16          |
| (2,1176) | 2:1755:A:LEU:HD12 | 2:1756:A:PRO:HD3  | 19       | 0.16          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 4        | 0.16          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 5        | 0.16          |
| (2,1135) | 2:1765:A:VAL:HG11 | 2:1804:A:PRO:HG2  | 6        | 0.16          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 15       | 0.16          |
| (2,1110) | 2:1747:A:GLN:HB2  | 2:1747:A:GLN:H    | 15       | 0.16          |
| (2,1103) | 2:1774:A:LYS:HE3  | 2:1774:A:LYS:HD3  | 8        | 0.16          |
| (2,1103) | 2:1774:A:LYS:HE3  | 2:1774:A:LYS:HD3  | 15       | 0.16          |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 1        | 0.16          |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 2        | 0.16          |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 4        | 0.16          |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 5        | 0.16          |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 14       | 0.16          |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 16       | 0.16          |
| (2,1093) | 2:1774:A:LYS:HA   | 2:1774:A:LYS:HG3  | 19       | 0.16          |
| (2,1079) | 2:1782:A:CYS:HA   | 2:1781:A:ILE:HG21 | 8        | 0.16          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 5        | 0.16          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 6        | 0.16          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 11       | 0.16          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 5        | 0.16          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 10       | 0.16          |
| (2,974)  | 2:1788:A:LEU:HA   | 2:1791:A:TYR:HB2  | 7        | 0.16          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD12 | 18       | 0.16          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 19       | 0.16          |
| (2,960)  | 2:1739:A:ILE:HD13 | 2:1735:A:ILE:HG23 | 8        | 0.16          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 1        | 0.16          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 2        | 0.16          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 10       | 0.16          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 12       | 0.16          |
| (2,917)  | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H    | 7        | 0.16          |
| (2,917)  | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H    | 9        | 0.16          |
| (2,917)  | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H    | 10       | 0.16          |
| (2,913)  | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2  | 18       | 0.16          |
| (2,903)  | 2:1768:A:THR:HA   | 2:1771:A:CYS:H    | 12       | 0.16          |
| (2,894)  | 2:1800:A:LYS:HA   | 2:1807:A:LEU:HD11 | 17       | 0.16          |
| (2,878)  | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 2        | 0.16          |
| (2,878)  | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 7        | 0.16          |
| (2,878)  | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 13       | 0.16          |
| (2,855)  | 2:1808:A:ASN:HB2  | 2:1809:A:ILE:H    | 11       | 0.16          |
| (2,846)  | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1  | 11       | 0.16          |
| (2,805)  | 2:1737:A:ARG:HD2  | 2:1737:A:ARG:H    | 18       | 0.16          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 14       | 0.16          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 2        | 0.16          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 7        | 0.16          |
| (2,723)  | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 12       | 0.16          |
| (2,722)  | 2:1804:A:PRO:HD3  | 2:1742:A:LEU:HD23 | 11       | 0.16          |
| (2,717)  | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H    | 6        | 0.16          |
| (2,717)  | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H    | 7        | 0.16          |
| (2,685)  | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG2  | 2        | 0.16          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 5        | 0.16          |
| (2,685)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG2  | 18       | 0.16          |
| (2,669)  | 1:120:B:ILE:HG22  | 1:117:B:ASP:H     | 18       | 0.16          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD2   | 3        | 0.16          |
| (2,576)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:H     | 7        | 0.16          |
| (2,576)  | 1:119:B:VAL:HG12  | 1:120:B:ILE:H     | 17       | 0.16          |
| (2,555)  | 1:124:B:ILE:HD12  | 1:124:B:ILE:HB    | 6        | 0.16          |
| (2,540)  | 1:134:B:ILE:HG23  | 2:1781:A:ILE:HA   | 15       | 0.16          |
| (2,526)  | 1:132:B:GLU:HG2   | 1:132:B:GLU:HA    | 3        | 0.16          |
| (2,525)  | 1:137:B:LEU:H     | 1:137:B:LEU:HD13  | 20       | 0.16          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,483)  | 1:126:B:LEU:HD23  | 1:127:B:GLU:H     | 12       | 0.16          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 9        | 0.16          |
| (2,463)  | 1:134:B:ILE:HD12  | 1:134:B:ILE:H     | 2        | 0.16          |
| (2,425)  | 1:138:B:MET:H     | 1:137:B:LEU:HD11  | 4        | 0.16          |
| (2,402)  | 1:141:B:ALA:H     | 1:140:B:PRO:HD2   | 2        | 0.16          |
| (2,389)  | 1:116:B:MET:H     | 1:115:B:GLN:HA    | 20       | 0.16          |
| (2,356)  | 1:121:B:ASP:H     | 1:121:B:ASP:HB3   | 14       | 0.16          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 4        | 0.16          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 7        | 0.16          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 13       | 0.16          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 19       | 0.16          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 20       | 0.16          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 7        | 0.16          |
| (2,155)  | 2:1771:A:CYS:HB2  | 2:1771:A:CYS:H    | 11       | 0.16          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 4        | 0.16          |
| (2,114)  | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 14       | 0.16          |
| (2,22)   | 2:1809:A:ILE:HG21 | 2:1809:A:ILE:H    | 20       | 0.16          |
| (1,35)   | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 8        | 0.16          |
| (3,36)   | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG3  | 14       | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 1        | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 5        | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 7        | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 8        | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD13 | 13       | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD12 | 15       | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD13 | 19       | 0.15          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG23 | 13       | 0.15          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 6        | 0.15          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 16       | 0.15          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 8        | 0.15          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 10       | 0.15          |
| (2,1721) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HG23 | 4        | 0.15          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB1  | 2        | 0.15          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB2  | 16       | 0.15          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 7        | 0.15          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 14       | 0.15          |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 8        | 0.15          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 10       | 0.15          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 17       | 0.15          |
| (2,1572) | 2:1809:A:ILE:HD12 | 2:1805:A:PHE:HD2  | 20       | 0.15          |
| (2,1570) | 2:1788:A:LEU:HD23 | 1:130:B:TYR:HE1   | 15       | 0.15          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 8        | 0.15          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 10       | 0.15          |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 20       | 0.15          |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 14       | 0.15          |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 11       | 0.15          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 1        | 0.15          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 10       | 0.15          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD12 | 19       | 0.15          |
| (2,1397) | 2:1793:A:ALA:HB3  | 2:1794:A:LYS:H    | 8        | 0.15          |
| (2,1397) | 2:1793:A:ALA:HB3  | 2:1794:A:LYS:H    | 17       | 0.15          |
| (2,1397) | 2:1793:A:ALA:HB2  | 2:1794:A:LYS:H    | 18       | 0.15          |
| (2,1376) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HA   | 6        | 0.15          |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 13       | 0.15          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 2        | 0.15          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 4        | 0.15          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 14       | 0.15          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 3        | 0.15          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 1        | 0.15          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 5        | 0.15          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB2  | 6        | 0.15          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 9        | 0.15          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 12       | 0.15          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 14       | 0.15          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG11 | 10       | 0.15          |
| (2,1293) | 2:1745:A:ALA:HB3  | 2:1746:A:ALA:H    | 1        | 0.15          |
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 3        | 0.15          |
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 11       | 0.15          |
| (2,1277) | 2:1780:A:PRO:HG3  | 1:134:B:ILE:HG22  | 3        | 0.15          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 15       | 0.15          |
| (2,1179) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:H    | 19       | 0.15          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 16       | 0.15          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 17       | 0.15          |
| (2,1136) | 2:1765:A:VAL:HG11 | 2:1766:A:GLN:H    | 15       | 0.15          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 8        | 0.15          |
| (2,1103) | 2:1774:A:LYS:HE3  | 2:1774:A:LYS:HD3  | 6        | 0.15          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 6        | 0.15          |
| (2,1100) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HG2  | 12       | 0.15          |
| (2,1079) | 2:1782:A:CYS:HA   | 2:1781:A:ILE:HG22 | 10       | 0.15          |
| (2,1079) | 2:1782:A:CYS:HA   | 2:1781:A:ILE:HG21 | 17       | 0.15          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 13       | 0.15          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 5        | 0.15          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 17       | 0.15          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 20       | 0.15          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1014) | 2:1733:A:LEU:HD23 | 2:1733:A:LEU:H    | 5        | 0.15          |
| (2,1014) | 2:1733:A:LEU:HD23 | 2:1733:A:LEU:H    | 16       | 0.15          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 6        | 0.15          |
| (2,969)  | 2:1769:A:LYS:HD3  | 2:1766:A:GLN:HA   | 12       | 0.15          |
| (2,969)  | 2:1769:A:LYS:HD3  | 2:1766:A:GLN:HA   | 17       | 0.15          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD12 | 6        | 0.15          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD12 | 7        | 0.15          |
| (2,960)  | 2:1739:A:ILE:HD12 | 2:1735:A:ILE:HG21 | 16       | 0.15          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 4        | 0.15          |
| (2,922)  | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 8        | 0.15          |
| (2,922)  | 2:1765:A:VAL:HG23 | 2:1804:A:PRO:HG2  | 12       | 0.15          |
| (2,917)  | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H    | 14       | 0.15          |
| (2,914)  | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 3        | 0.15          |
| (2,914)  | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 5        | 0.15          |
| (2,914)  | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 14       | 0.15          |
| (2,906)  | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA   | 8        | 0.15          |
| (2,903)  | 2:1768:A:THR:HA   | 2:1771:A:CYS:H    | 9        | 0.15          |
| (2,889)  | 2:1741:A:SER:HB3  | 2:1761:A:MET:HG3  | 2        | 0.15          |
| (2,846)  | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1  | 13       | 0.15          |
| (2,806)  | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H    | 6        | 0.15          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 1        | 0.15          |
| (2,803)  | 2:1731:A:ARG:HD2  | 2:1731:A:ARG:HA   | 7        | 0.15          |
| (2,754)  | 2:1774:A:LYS:HG2  | 2:1774:A:LYS:HE3  | 13       | 0.15          |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 5        | 0.15          |
| (2,749)  | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H    | 9        | 0.15          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 4        | 0.15          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 11       | 0.15          |
| (2,742)  | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 15       | 0.15          |
| (2,717)  | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H    | 1        | 0.15          |
| (2,717)  | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H    | 5        | 0.15          |
| (2,717)  | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H    | 8        | 0.15          |
| (2,717)  | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H    | 15       | 0.15          |
| (2,717)  | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H    | 19       | 0.15          |
| (2,685)  | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG2  | 19       | 0.15          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 11       | 0.15          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 16       | 0.15          |
| (2,652)  | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1   | 17       | 0.15          |
| (2,598)  | 1:116:B:MET:HA    | 1:116:B:MET:HG3   | 16       | 0.15          |
| (2,576)  | 1:119:B:VAL:HG11  | 1:120:B:ILE:H     | 8        | 0.15          |
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 2        | 0.15          |
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 9        | 0.15          |
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG22  | 18       | 0.15          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 20       | 0.15          |
| (2,569)  | 1:124:B:ILE:HA    | 1:124:B:ILE:HG22  | 7        | 0.15          |
| (2,569)  | 1:124:B:ILE:HA    | 1:124:B:ILE:HG23  | 11       | 0.15          |
| (2,569)  | 1:124:B:ILE:HA    | 1:124:B:ILE:HG22  | 19       | 0.15          |
| (2,555)  | 1:124:B:ILE:HD11  | 1:124:B:ILE:HB    | 5        | 0.15          |
| (2,543)  | 1:134:B:ILE:HG12  | 1:134:B:ILE:HA    | 2        | 0.15          |
| (2,543)  | 1:134:B:ILE:HG12  | 1:134:B:ILE:HA    | 9        | 0.15          |
| (2,543)  | 1:134:B:ILE:HG12  | 1:134:B:ILE:HA    | 19       | 0.15          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 15       | 0.15          |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG22  | 1        | 0.15          |
| (2,495)  | 1:133:B:GLU:HB3   | 1:134:B:ILE:HG21  | 13       | 0.15          |
| (2,483)  | 1:126:B:LEU:HD21  | 1:127:B:GLU:H     | 2        | 0.15          |
| (2,483)  | 1:126:B:LEU:HD22  | 1:127:B:GLU:H     | 19       | 0.15          |
| (2,415)  | 1:123:B:ILE:H     | 1:122:B:ASP:HB2   | 8        | 0.15          |
| (2,394)  | 1:117:B:ASP:H     | 1:116:B:MET:HB2   | 2        | 0.15          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 3        | 0.15          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 10       | 0.15          |
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 3        | 0.15          |
| (2,205)  | 2:1785:A:LEU:H    | 2:1784:A:GLN:HG2  | 18       | 0.15          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 8        | 0.15          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 9        | 0.15          |
| (2,114)  | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H    | 16       | 0.15          |
| (1,35)   | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 18       | 0.15          |
| (1,24)   | 2:1769:A:LYS:H    | 2:1765:A:VAL:O    | 9        | 0.15          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 6        | 0.14          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD13 | 10       | 0.14          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD13 | 11       | 0.14          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 12       | 0.14          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD12 | 17       | 0.14          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD13 | 20       | 0.14          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG21 | 3        | 0.14          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 15       | 0.14          |
| (3,12)   | 1:123:B:ILE:HA    | 1:126:B:LEU:HD22  | 3        | 0.14          |
| (3,12)   | 1:123:B:ILE:HA    | 1:126:B:LEU:HD21  | 14       | 0.14          |
| (3,9)    | 1:120:B:ILE:HG23  | 1:120:B:ILE:HG12  | 4        | 0.14          |
| (3,9)    | 1:120:B:ILE:HG21  | 1:120:B:ILE:HG12  | 6        | 0.14          |
| (3,9)    | 1:120:B:ILE:HG22  | 1:120:B:ILE:HG12  | 11       | 0.14          |
| (3,9)    | 1:120:B:ILE:HG22  | 1:120:B:ILE:HG12  | 19       | 0.14          |
| (3,9)    | 1:120:B:ILE:HG21  | 1:120:B:ILE:HG12  | 20       | 0.14          |
| (2,1740) | 2:1791:A:TYR:HE1  | 2:1739:A:ILE:HB   | 3        | 0.14          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 16       | 0.14          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 17       | 0.14          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 1        | 0.14          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 14       | 0.14          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 17       | 0.14          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 2        | 0.14          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD2  | 14       | 0.14          |
| (2,1698) | 2:1788:A:LEU:HD23 | 2:1787:A:ALA:H    | 11       | 0.14          |
| (2,1654) | 2:1809:A:ILE:HG21 | 2:1810:A:LYS:HG3  | 20       | 0.14          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB1  | 7        | 0.14          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 4        | 0.14          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 19       | 0.14          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 8        | 0.14          |
| (2,1595) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HE22 | 19       | 0.14          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 18       | 0.14          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 3        | 0.14          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 5        | 0.14          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 20       | 0.14          |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 1        | 0.14          |
| (2,1514) | 2:1764:A:VAL:HG11 | 2:1781:A:ILE:HG21 | 13       | 0.14          |
| (2,1476) | 2:1805:A:PHE:HB3  | 2:1809:A:ILE:HD11 | 16       | 0.14          |
| (2,1432) | 2:1783:A:LYS:HB2  | 2:1783:A:LYS:HE2  | 8        | 0.14          |
| (2,1428) | 2:1790:A:ALA:HB2  | 2:1809:A:ILE:HD11 | 13       | 0.14          |
| (2,1428) | 2:1790:A:ALA:HB3  | 2:1809:A:ILE:HD11 | 14       | 0.14          |
| (2,1414) | 2:1735:A:ILE:HD11 | 1:130:B:TYR:HB3   | 6        | 0.14          |
| (2,1397) | 2:1793:A:ALA:HB1  | 2:1794:A:LYS:H    | 6        | 0.14          |
| (2,1376) | 2:1809:A:ILE:HG22 | 2:1810:A:LYS:HA   | 9        | 0.14          |
| (2,1371) | 2:1764:A:VAL:HG22 | 2:1764:A:VAL:H    | 20       | 0.14          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 2        | 0.14          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 5        | 0.14          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 18       | 0.14          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 19       | 0.14          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 20       | 0.14          |
| (2,1331) | 2:1811:A:GLN:HB3  | 2:1811:A:GLN:H    | 10       | 0.14          |
| (2,1310) | 2:1789:A:ALA:HA   | 2:1792:A:HIS:HB2  | 3        | 0.14          |
| (2,1304) | 2:1751:A:ALA:HB3  | 2:1752:A:ASN:HB2  | 1        | 0.14          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB3  | 8        | 0.14          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB2  | 13       | 0.14          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB2  | 15       | 0.14          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB2  | 16       | 0.14          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 17       | 0.14          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 18       | 0.14          |
| (2,1293) | 2:1745:A:ALA:HB3  | 2:1746:A:ALA:H    | 7        | 0.14          |
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 16       | 0.14          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 18       | 0.14          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 8        | 0.14          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 4        | 0.14          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 8        | 0.14          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 11       | 0.14          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 20       | 0.14          |
| (2,1179) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:H    | 18       | 0.14          |
| (2,1171) | 2:1760:A:LYS:HB2  | 2:1759:A:GLN:HE21 | 2        | 0.14          |
| (2,1169) | 2:1741:A:SER:HA   | 2:1744:A:HIS:H    | 20       | 0.14          |
| (2,1156) | 2:1743:A:VAL:HG22 | 2:1747:A:GLN:HE22 | 7        | 0.14          |
| (2,1146) | 2:1788:A:LEU:HD21 | 2:1735:A:ILE:HA   | 20       | 0.14          |
| (2,1119) | 2:1739:A:ILE:HG22 | 2:1736:A:GLN:HA   | 5        | 0.14          |
| (2,1119) | 2:1739:A:ILE:HG21 | 2:1736:A:GLN:HA   | 6        | 0.14          |
| (2,1102) | 2:1774:A:LYS:HD2  | 2:1774:A:LYS:HE3  | 17       | 0.14          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 6        | 0.14          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 11       | 0.14          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 1        | 0.14          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 4        | 0.14          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 7        | 0.14          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 13       | 0.14          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 15       | 0.14          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 16       | 0.14          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 15       | 0.14          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 9        | 0.14          |
| (2,1014) | 2:1733:A:LEU:HD22 | 2:1733:A:LEU:H    | 14       | 0.14          |
| (2,1006) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HB3  | 6        | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 5        | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 6        | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 9        | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 10       | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 11       | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 14       | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 15       | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 16       | 0.14          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 20       | 0.14          |
| (2,979)  | 2:1757:A:SER:HA   | 2:1760:A:LYS:HB2  | 9        | 0.14          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 5        | 0.14          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD12 | 11       | 0.14          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 17       | 0.14          |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD13 | 20       | 0.14          |
| (2,963)  | 2:1739:A:ILE:HD13 | 2:1792:A:HIS:HB3  | 14       | 0.14          |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 11       | 0.14          |

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| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (2,951) | 2:1780:A:PRO:HB3  | 1:134:B:ILE:HG22 | 13       | 0.14          |
| (2,948) | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2 | 20       | 0.14          |
| (2,922) | 2:1765:A:VAL:HG23 | 2:1804:A:PRO:HG2 | 3        | 0.14          |
| (2,922) | 2:1765:A:VAL:HG23 | 2:1804:A:PRO:HG2 | 19       | 0.14          |
| (2,917) | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H   | 17       | 0.14          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2 | 8        | 0.14          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2 | 18       | 0.14          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2 | 19       | 0.14          |
| (2,913) | 2:1769:A:LYS:HA   | 2:1769:A:LYS:HG2 | 7        | 0.14          |
| (2,906) | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA  | 11       | 0.14          |
| (2,906) | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA  | 14       | 0.14          |
| (2,903) | 2:1768:A:THR:HA   | 2:1771:A:CYS:H   | 2        | 0.14          |
| (2,903) | 2:1768:A:THR:HA   | 2:1771:A:CYS:H   | 8        | 0.14          |
| (2,903) | 2:1768:A:THR:HA   | 2:1771:A:CYS:H   | 16       | 0.14          |
| (2,903) | 2:1768:A:THR:HA   | 2:1771:A:CYS:H   | 17       | 0.14          |
| (2,882) | 2:1807:A:LEU:HG   | 2:1807:A:LEU:H   | 13       | 0.14          |
| (2,882) | 2:1807:A:LEU:HG   | 2:1807:A:LEU:H   | 19       | 0.14          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 1        | 0.14          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 10       | 0.14          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 16       | 0.14          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 17       | 0.14          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 19       | 0.14          |
| (2,868) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HG2 | 18       | 0.14          |
| (2,806) | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H   | 17       | 0.14          |
| (2,757) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H   | 12       | 0.14          |
| (2,749) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H   | 3        | 0.14          |
| (2,742) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 1        | 0.14          |
| (2,742) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 8        | 0.14          |
| (2,723) | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H   | 10       | 0.14          |
| (2,723) | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H   | 14       | 0.14          |
| (2,723) | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H   | 16       | 0.14          |
| (2,717) | 2:1790:A:ALA:HB2  | 2:1790:A:ALA:H   | 4        | 0.14          |
| (2,717) | 2:1790:A:ALA:HB2  | 2:1790:A:ALA:H   | 9        | 0.14          |
| (2,717) | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H   | 10       | 0.14          |
| (2,717) | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H   | 13       | 0.14          |
| (2,717) | 2:1790:A:ALA:HB2  | 2:1790:A:ALA:H   | 14       | 0.14          |
| (2,717) | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H   | 17       | 0.14          |
| (2,717) | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H   | 18       | 0.14          |
| (2,645) | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1  | 9        | 0.14          |
| (2,638) | 1:115:B:GLN:HG2   | 1:115:B:GLN:HA   | 2        | 0.14          |
| (2,593) | 1:131:B:ASN:HB3   | 1:134:B:ILE:HG21 | 6        | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23 | 1        | 0.14          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 4        | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG21  | 6        | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 8        | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 12       | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG22  | 14       | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG21  | 16       | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG22  | 17       | 0.14          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG21  | 19       | 0.14          |
| (2,560) | 1:134:B:ILE:HD12  | 1:131:B:ASN:HD22  | 7        | 0.14          |
| (2,543) | 1:134:B:ILE:HG12  | 1:134:B:ILE:HA    | 3        | 0.14          |
| (2,543) | 1:134:B:ILE:HG12  | 1:134:B:ILE:HA    | 8        | 0.14          |
| (2,522) | 1:135:B:LEU:HD13  | 1:135:B:LEU:HA    | 14       | 0.14          |
| (2,500) | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 10       | 0.14          |
| (2,500) | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 11       | 0.14          |
| (2,500) | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 16       | 0.14          |
| (2,500) | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 18       | 0.14          |
| (2,499) | 1:126:B:LEU:HG    | 1:126:B:LEU:H     | 18       | 0.14          |
| (2,487) | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 14       | 0.14          |
| (2,483) | 1:126:B:LEU:HD22  | 1:127:B:GLU:H     | 17       | 0.14          |
| (2,471) | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 12       | 0.14          |
| (2,431) | 1:125:B:SER:H     | 1:124:B:ILE:HG12  | 18       | 0.14          |
| (2,400) | 1:141:B:ALA:H     | 1:140:B:PRO:HA    | 6        | 0.14          |
| (2,389) | 1:116:B:MET:H     | 1:115:B:GLN:HA    | 9        | 0.14          |
| (2,333) | 1:137:B:LEU:H     | 1:136:B:GLY:H     | 15       | 0.14          |
| (2,333) | 1:137:B:LEU:H     | 1:136:B:GLY:H     | 18       | 0.14          |
| (2,321) | 2:1777:A:GLY:H    | 2:1776:A:ASN:HA   | 5        | 0.14          |
| (2,289) | 2:1784:A:GLN:HE21 | 2:1784:A:GLN:HB3  | 5        | 0.14          |
| (2,239) | 2:1779:A:CYS:H    | 2:1773:A:ARG:HB3  | 8        | 0.14          |
| (2,238) | 2:1779:A:CYS:H    | 2:1773:A:ARG:HD3  | 13       | 0.14          |
| (2,130) | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 1        | 0.14          |
| (2,130) | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 7        | 0.14          |
| (2,108) | 2:1741:A:SER:H    | 2:1761:A:MET:HE3  | 11       | 0.14          |
| (1,45)  | 1:126:B:LEU:O     | 1:130:B:TYR:H     | 3        | 0.14          |
| (3,36)  | 2:1745:A:ALA:HB2  | 2:1761:A:MET:HG3  | 9        | 0.13          |
| (3,36)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG3  | 11       | 0.13          |
| (3,36)  | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG3  | 15       | 0.13          |
| (3,30)  | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HD2  | 7        | 0.13          |
| (3,30)  | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HB2  | 10       | 0.13          |
| (3,22)  | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD12 | 4        | 0.13          |
| (3,22)  | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 14       | 0.13          |
| (3,22)  | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD12 | 16       | 0.13          |
| (3,18)  | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG22 | 14       | 0.13          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (3,9)    | 1:120:B:ILE:HG22  | 1:120:B:ILE:HG12  | 2        | 0.13          |
| (3,9)    | 1:120:B:ILE:HG22  | 1:120:B:ILE:HG12  | 18       | 0.13          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 1        | 0.13          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 6        | 0.13          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 8        | 0.13          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 1        | 0.13          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 4        | 0.13          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 6        | 0.13          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 12       | 0.13          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 13       | 0.13          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 20       | 0.13          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 15       | 0.13          |
| (2,1681) | 2:1739:A:ILE:HG22 | 2:1740:A:GLN:HG3  | 2        | 0.13          |
| (2,1621) | 2:1774:A:LYS:HD3  | 2:1805:A:PHE:HE2  | 5        | 0.13          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 16       | 0.13          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 7        | 0.13          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 14       | 0.13          |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 11       | 0.13          |
| (2,1572) | 2:1809:A:ILE:HD13 | 2:1805:A:PHE:HD1  | 11       | 0.13          |
| (2,1537) | 2:1765:A:VAL:HG23 | 2:1765:A:VAL:HA   | 9        | 0.13          |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 11       | 0.13          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 2        | 0.13          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 7        | 0.13          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 16       | 0.13          |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 4        | 0.13          |
| (2,1508) | 2:1789:A:ALA:HB3  | 2:1786:A:ILE:HA   | 3        | 0.13          |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD12 | 10       | 0.13          |
| (2,1440) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HE2  | 20       | 0.13          |
| (2,1397) | 2:1793:A:ALA:HB2  | 2:1794:A:LYS:H    | 12       | 0.13          |
| (2,1397) | 2:1793:A:ALA:HB1  | 2:1794:A:LYS:H    | 15       | 0.13          |
| (2,1379) | 2:1809:A:ILE:HG21 | 2:1793:A:ALA:HB2  | 3        | 0.13          |
| (2,1371) | 2:1764:A:VAL:HG21 | 2:1764:A:VAL:H    | 15       | 0.13          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 7        | 0.13          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 11       | 0.13          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 13       | 0.13          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 15       | 0.13          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 16       | 0.13          |
| (2,1334) | 2:1772:A:LYS:HB3  | 2:1772:A:LYS:HA   | 1        | 0.13          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 4        | 0.13          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB3  | 10       | 0.13          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB1  | 11       | 0.13          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB2  | 20       | 0.13          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1299) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG21 | 18       | 0.13          |
| (2,1281) | 2:1736:A:GLN:HG2  | 2:1736:A:GLN:H    | 13       | 0.13          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 2        | 0.13          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 3        | 0.13          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 8        | 0.13          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 9        | 0.13          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 15       | 0.13          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 17       | 0.13          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 18       | 0.13          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 4        | 0.13          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 6        | 0.13          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 3        | 0.13          |
| (2,1219) | 2:1800:A:LYS:HG3  | 2:1800:A:LYS:HE2  | 3        | 0.13          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 1        | 0.13          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 3        | 0.13          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 5        | 0.13          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 10       | 0.13          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 12       | 0.13          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 14       | 0.13          |
| (2,1179) | 2:1755:A:LEU:HD12 | 2:1755:A:LEU:H    | 15       | 0.13          |
| (2,1168) | 2:1724:A:THR:HA   | 2:1724:A:THR:HG21 | 4        | 0.13          |
| (2,1146) | 2:1788:A:LEU:HD21 | 2:1735:A:ILE:HA   | 6        | 0.13          |
| (2,1131) | 2:1761:A:MET:HE1  | 2:1742:A:LEU:H    | 12       | 0.13          |
| (2,1127) | 2:1761:A:MET:HE1  | 2:1738:A:ALA:HB1  | 18       | 0.13          |
| (2,1119) | 2:1739:A:ILE:HG21 | 2:1736:A:GLN:HA   | 1        | 0.13          |
| (2,1119) | 2:1739:A:ILE:HG22 | 2:1736:A:GLN:HA   | 3        | 0.13          |
| (2,1105) | 2:1774:A:LYS:HE3  | 2:1805:A:PHE:HE1  | 15       | 0.13          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 2        | 0.13          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 8        | 0.13          |
| (2,1058) | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:H    | 16       | 0.13          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 16       | 0.13          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 9        | 0.13          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 12       | 0.13          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 14       | 0.13          |
| (2,1014) | 2:1733:A:LEU:HD23 | 2:1733:A:LEU:H    | 13       | 0.13          |
| (2,1014) | 2:1733:A:LEU:HD22 | 2:1733:A:LEU:H    | 19       | 0.13          |
| (2,1006) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HB3  | 14       | 0.13          |
| (2,1006) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HB3  | 17       | 0.13          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 1        | 0.13          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 2        | 0.13          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 18       | 0.13          |
| (2,992)  | 2:1794:A:LYS:HD2  | 2:1794:A:LYS:HA   | 13       | 0.13          |

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| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (2,969) | 2:1769:A:LYS:HD3  | 2:1766:A:GLN:HA  | 7        | 0.13          |
| (2,953) | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H   | 8        | 0.13          |
| (2,953) | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H   | 14       | 0.13          |
| (2,922) | 2:1765:A:VAL:HG22 | 2:1804:A:PRO:HG2 | 6        | 0.13          |
| (2,917) | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H   | 1        | 0.13          |
| (2,917) | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H   | 16       | 0.13          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2 | 4        | 0.13          |
| (2,906) | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA  | 4        | 0.13          |
| (2,906) | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA  | 6        | 0.13          |
| (2,906) | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA  | 12       | 0.13          |
| (2,906) | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA  | 15       | 0.13          |
| (2,898) | 2:1739:A:ILE:HG12 | 2:1739:A:ILE:H   | 9        | 0.13          |
| (2,882) | 2:1807:A:LEU:HG   | 2:1807:A:LEU:H   | 20       | 0.13          |
| (2,881) | 2:1807:A:LEU:HG   | 2:1801:A:CYS:HB2 | 8        | 0.13          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 4        | 0.13          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 5        | 0.13          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 6        | 0.13          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 12       | 0.13          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 15       | 0.13          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H   | 20       | 0.13          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB3 | 1        | 0.13          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB3 | 2        | 0.13          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB2 | 14       | 0.13          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1 | 15       | 0.13          |
| (2,806) | 2:1731:A:ARG:HD2  | 2:1735:A:ILE:H   | 7        | 0.13          |
| (2,757) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:H   | 8        | 0.13          |
| (2,749) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:H   | 16       | 0.13          |
| (2,742) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H   | 9        | 0.13          |
| (2,717) | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H   | 11       | 0.13          |
| (2,717) | 2:1790:A:ALA:HB3  | 2:1790:A:ALA:H   | 12       | 0.13          |
| (2,717) | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H   | 20       | 0.13          |
| (2,652) | 1:127:B:GLU:HA    | 1:130:B:TYR:HD2  | 5        | 0.13          |
| (2,652) | 1:127:B:GLU:HA    | 1:130:B:TYR:HD1  | 14       | 0.13          |
| (2,645) | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE2  | 8        | 0.13          |
| (2,645) | 1:132:B:GLU:HB2   | 1:130:B:TYR:HE1  | 11       | 0.13          |
| (2,636) | 1:135:B:LEU:HD22  | 1:132:B:GLU:HB2  | 15       | 0.13          |
| (2,598) | 1:116:B:MET:HA    | 1:116:B:MET:HG3  | 17       | 0.13          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23 | 5        | 0.13          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG21 | 7        | 0.13          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23 | 10       | 0.13          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23 | 11       | 0.13          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23 | 13       | 0.13          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,571)  | 1:123:B:ILE:HB    | 1:123:B:ILE:HG23  | 15       | 0.13          |
| (2,509)  | 1:117:B:ASP:HA    | 1:117:B:ASP:HB3   | 10       | 0.13          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 6        | 0.13          |
| (2,500)  | 1:135:B:LEU:HG    | 1:135:B:LEU:H     | 12       | 0.13          |
| (2,487)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 4        | 0.13          |
| (2,487)  | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 18       | 0.13          |
| (2,483)  | 1:126:B:LEU:HD21  | 1:127:B:GLU:H     | 4        | 0.13          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 4        | 0.13          |
| (2,471)  | 1:124:B:ILE:H     | 1:123:B:ILE:HG23  | 11       | 0.13          |
| (2,470)  | 1:125:B:SER:H     | 1:124:B:ILE:HG22  | 2        | 0.13          |
| (2,448)  | 1:131:B:ASN:H     | 1:131:B:ASN:HD21  | 8        | 0.13          |
| (2,448)  | 1:131:B:ASN:H     | 1:131:B:ASN:HD21  | 19       | 0.13          |
| (2,427)  | 1:136:B:GLY:H     | 1:135:B:LEU:HG    | 11       | 0.13          |
| (2,389)  | 1:116:B:MET:H     | 1:115:B:GLN:HA    | 12       | 0.13          |
| (2,386)  | 1:126:B:LEU:H     | 1:126:B:LEU:HD13  | 1        | 0.13          |
| (2,338)  | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 17       | 0.13          |
| (2,321)  | 2:1777:A:GLY:H    | 2:1776:A:ASN:HA   | 3        | 0.13          |
| (2,291)  | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 4        | 0.13          |
| (2,130)  | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 6        | 0.13          |
| (2,7)    | 2:1785:A:LEU:H    | 2:1784:A:GLN:HB2  | 5        | 0.13          |
| (2,7)    | 2:1785:A:LEU:H    | 2:1784:A:GLN:HB2  | 12       | 0.13          |
| (1,35)   | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 9        | 0.13          |
| (1,24)   | 2:1769:A:LYS:H    | 2:1765:A:VAL:O    | 16       | 0.13          |
| (1,24)   | 2:1769:A:LYS:H    | 2:1765:A:VAL:O    | 17       | 0.13          |
| (3,36)   | 2:1745:A:ALA:HB1  | 2:1761:A:MET:HG3  | 20       | 0.12          |
| (3,30)   | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HD2  | 1        | 0.12          |
| (3,30)   | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HD2  | 11       | 0.12          |
| (3,30)   | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HB2  | 17       | 0.12          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD11 | 9        | 0.12          |
| (3,22)   | 2:1733:A:LEU:HG   | 2:1733:A:LEU:HD13 | 18       | 0.12          |
| (3,18)   | 2:1743:A:VAL:HA   | 2:1743:A:VAL:HG21 | 19       | 0.12          |
| (3,9)    | 1:120:B:ILE:HG23  | 1:120:B:ILE:HG12  | 5        | 0.12          |
| (3,9)    | 1:120:B:ILE:HG21  | 1:120:B:ILE:HG12  | 14       | 0.12          |
| (3,9)    | 1:120:B:ILE:HG21  | 1:120:B:ILE:HG12  | 16       | 0.12          |
| (2,1740) | 2:1791:A:TYR:HE2  | 2:1739:A:ILE:HB   | 9        | 0.12          |
| (2,1733) | 2:1758:A:CYS:HB3  | 2:1744:A:HIS:HD2  | 6        | 0.12          |
| (2,1728) | 2:1791:A:TYR:HA   | 2:1791:A:TYR:HD1  | 9        | 0.12          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 2        | 0.12          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 3        | 0.12          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 7        | 0.12          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 18       | 0.12          |
| (2,1717) | 2:1805:A:PHE:HD2  | 2:1804:A:PRO:HB2  | 18       | 0.12          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1716) | 2:1785:A:LEU:HB2  | 2:1805:A:PHE:HE1  | 1        | 0.12          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 3        | 0.12          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 13       | 0.12          |
| (2,1698) | 2:1788:A:LEU:HD22 | 2:1787:A:ALA:H    | 15       | 0.12          |
| (2,1664) | 2:1811:A:GLN:HG3  | 2:1811:A:GLN:H    | 12       | 0.12          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 1        | 0.12          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 12       | 0.12          |
| (2,1619) | 2:1760:A:LYS:HD3  | 2:1760:A:LYS:HA   | 13       | 0.12          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 6        | 0.12          |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 6        | 0.12          |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 15       | 0.12          |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 16       | 0.12          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 8        | 0.12          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 9        | 0.12          |
| (2,1574) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HB2  | 11       | 0.12          |
| (2,1523) | 2:1766:A:GLN:HA   | 2:1766:A:GLN:HG2  | 3        | 0.12          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 13       | 0.12          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 15       | 0.12          |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 6        | 0.12          |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 10       | 0.12          |
| (2,1511) | 2:1738:A:ALA:HB2  | 2:1735:A:ILE:HA   | 8        | 0.12          |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 6        | 0.12          |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 8        | 0.12          |
| (2,1497) | 2:1766:A:GLN:HB3  | 2:1763:A:ARG:HA   | 9        | 0.12          |
| (2,1471) | 2:1798:A:GLU:HA   | 2:1798:A:GLU:HG2  | 19       | 0.12          |
| (2,1440) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HE2  | 11       | 0.12          |
| (2,1428) | 2:1790:A:ALA:HB1  | 2:1809:A:ILE:HD13 | 7        | 0.12          |
| (2,1397) | 2:1793:A:ALA:HB2  | 2:1794:A:LYS:H    | 4        | 0.12          |
| (2,1385) | 2:1785:A:LEU:HD12 | 2:1768:A:THR:HG21 | 18       | 0.12          |
| (2,1383) | 2:1785:A:LEU:HD13 | 2:1785:A:LEU:HA   | 15       | 0.12          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 11       | 0.12          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 14       | 0.12          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 4        | 0.12          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 14       | 0.12          |
| (2,1351) | 2:1732:A:ARG:HG3  | 2:1732:A:ARG:H    | 17       | 0.12          |
| (2,1342) | 2:1756:A:PRO:HD2  | 2:1756:A:PRO:HA   | 9        | 0.12          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB3  | 3        | 0.12          |
| (2,1299) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG21 | 7        | 0.12          |
| (2,1298) | 2:1761:A:MET:HA   | 2:1764:A:VAL:HG13 | 6        | 0.12          |
| (2,1293) | 2:1745:A:ALA:HB1  | 2:1746:A:ALA:H    | 5        | 0.12          |
| (2,1293) | 2:1745:A:ALA:HB2  | 2:1746:A:ALA:H    | 14       | 0.12          |
| (2,1293) | 2:1745:A:ALA:HB2  | 2:1746:A:ALA:H    | 19       | 0.12          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1281) | 2:1736:A:GLN:HG2  | 2:1736:A:GLN:H    | 9        | 0.12          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 1        | 0.12          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 4        | 0.12          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 10       | 0.12          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 11       | 0.12          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 13       | 0.12          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 16       | 0.12          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 2        | 0.12          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 9        | 0.12          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 14       | 0.12          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 16       | 0.12          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 1        | 0.12          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 2        | 0.12          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 4        | 0.12          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 13       | 0.12          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 20       | 0.12          |
| (2,1200) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:H    | 20       | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 2        | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 6        | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 7        | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 9        | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 13       | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 16       | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 17       | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 18       | 0.12          |
| (2,1194) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:HA   | 19       | 0.12          |
| (2,1179) | 2:1755:A:LEU:HD11 | 2:1755:A:LEU:H    | 16       | 0.12          |
| (2,1169) | 2:1741:A:SER:HA   | 2:1744:A:HIS:H    | 1        | 0.12          |
| (2,1168) | 2:1724:A:THR:HA   | 2:1724:A:THR:HG22 | 14       | 0.12          |
| (2,1148) | 2:1788:A:LEU:HD21 | 1:130:B:TYR:HD2   | 20       | 0.12          |
| (2,1117) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:H    | 13       | 0.12          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 15       | 0.12          |
| (2,1104) | 2:1774:A:LYS:HG3  | 2:1774:A:LYS:HE3  | 16       | 0.12          |
| (2,1099) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HD3  | 17       | 0.12          |
| (2,1092) | 2:1774:A:LYS:HA   | 2:1774:A:LYS:HG2  | 1        | 0.12          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 18       | 0.12          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 3        | 0.12          |
| (2,1022) | 2:1796:A:CYS:HB3  | 2:1796:A:CYS:H    | 12       | 0.12          |
| (2,1014) | 2:1733:A:LEU:HD22 | 2:1733:A:LEU:H    | 7        | 0.12          |
| (2,999)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HB2  | 19       | 0.12          |
| (2,979)  | 2:1757:A:SER:HA   | 2:1760:A:LYS:HB2  | 12       | 0.12          |
| (2,979)  | 2:1757:A:SER:HA   | 2:1760:A:LYS:HB2  | 14       | 0.12          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (2,964) | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD11 | 3        | 0.12          |
| (2,964) | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD13 | 13       | 0.12          |
| (2,954) | 2:1779:A:CYS:HB3  | 2:1774:A:LYS:HD3  | 17       | 0.12          |
| (2,953) | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 5        | 0.12          |
| (2,953) | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 6        | 0.12          |
| (2,922) | 2:1765:A:VAL:HG21 | 2:1804:A:PRO:HG2  | 1        | 0.12          |
| (2,922) | 2:1765:A:VAL:HG23 | 2:1804:A:PRO:HG2  | 5        | 0.12          |
| (2,922) | 2:1765:A:VAL:HG22 | 2:1804:A:PRO:HG2  | 15       | 0.12          |
| (2,917) | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H    | 8        | 0.12          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 10       | 0.12          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 12       | 0.12          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 13       | 0.12          |
| (2,914) | 2:1760:A:LYS:HG2  | 2:1760:A:LYS:HB2  | 15       | 0.12          |
| (2,903) | 2:1768:A:THR:HA   | 2:1771:A:CYS:H    | 1        | 0.12          |
| (2,903) | 2:1768:A:THR:HA   | 2:1771:A:CYS:H    | 4        | 0.12          |
| (2,889) | 2:1741:A:SER:HB3  | 2:1761:A:MET:HG3  | 13       | 0.12          |
| (2,882) | 2:1807:A:LEU:HG   | 2:1807:A:LEU:H    | 3        | 0.12          |
| (2,878) | 2:1731:A:ARG:HA   | 2:1735:A:ILE:H    | 9        | 0.12          |
| (2,868) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HG2  | 7        | 0.12          |
| (2,863) | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HB3  | 17       | 0.12          |
| (2,863) | 2:1773:A:ARG:HA   | 2:1773:A:ARG:HB3  | 19       | 0.12          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1  | 3        | 0.12          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB3  | 7        | 0.12          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB2  | 9        | 0.12          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB3  | 10       | 0.12          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1  | 16       | 0.12          |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1  | 18       | 0.12          |
| (2,826) | 2:1791:A:TYR:HA   | 2:1794:A:LYS:HB2  | 12       | 0.12          |
| (2,826) | 2:1791:A:TYR:HA   | 2:1794:A:LYS:HB2  | 13       | 0.12          |
| (2,765) | 2:1810:A:LYS:HB3  | 2:1810:A:LYS:HE2  | 5        | 0.12          |
| (2,763) | 2:1810:A:LYS:HE2  | 2:1810:A:LYS:H    | 18       | 0.12          |
| (2,746) | 2:1783:A:LYS:HG3  | 2:1783:A:LYS:H    | 10       | 0.12          |
| (2,742) | 2:1760:A:LYS:HE2  | 2:1760:A:LYS:H    | 7        | 0.12          |
| (2,723) | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 4        | 0.12          |
| (2,723) | 2:1804:A:PRO:HA   | 2:1806:A:CYS:H    | 9        | 0.12          |
| (2,717) | 2:1790:A:ALA:HB1  | 2:1790:A:ALA:H    | 2        | 0.12          |
| (2,668) | 1:120:B:ILE:HD13  | 1:116:B:MET:HA    | 6        | 0.12          |
| (2,647) | 1:133:B:GLU:HB3   | 1:131:B:ASN:HD22  | 12       | 0.12          |
| (2,598) | 1:116:B:MET:HA    | 1:116:B:MET:HG3   | 18       | 0.12          |
| (2,571) | 1:123:B:ILE:HB    | 1:123:B:ILE:HG21  | 3        | 0.12          |
| (2,569) | 1:124:B:ILE:HA    | 1:124:B:ILE:HG23  | 13       | 0.12          |
| (2,569) | 1:124:B:ILE:HA    | 1:124:B:ILE:HG22  | 17       | 0.12          |

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| Key      | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|----------|------------------|-------------------|----------|---------------|
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD13  | 1        | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD11  | 8        | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD13  | 10       | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD12  | 11       | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD12  | 13       | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD13  | 14       | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD11  | 15       | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD12  | 17       | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD13  | 18       | 0.12          |
| (2,557)  | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD12  | 19       | 0.12          |
| (2,543)  | 1:134:B:ILE:HG12 | 1:134:B:ILE:HA    | 4        | 0.12          |
| (2,511)  | 1:119:B:VAL:H    | 1:118:B:ASP:HA    | 3        | 0.12          |
| (2,509)  | 1:117:B:ASP:HA   | 1:117:B:ASP:HB3   | 3        | 0.12          |
| (2,509)  | 1:117:B:ASP:HA   | 1:117:B:ASP:HB3   | 8        | 0.12          |
| (2,501)  | 1:120:B:ILE:HG12 | 1:120:B:ILE:HA    | 1        | 0.12          |
| (2,500)  | 1:135:B:LEU:HG   | 1:135:B:LEU:H     | 13       | 0.12          |
| (2,500)  | 1:135:B:LEU:HG   | 1:135:B:LEU:H     | 14       | 0.12          |
| (2,495)  | 1:133:B:GLU:HB3  | 1:134:B:ILE:HG21  | 6        | 0.12          |
| (2,495)  | 1:133:B:GLU:HB3  | 1:134:B:ILE:HG23  | 7        | 0.12          |
| (2,487)  | 1:117:B:ASP:HB3  | 1:120:B:ILE:HB    | 2        | 0.12          |
| (2,487)  | 1:117:B:ASP:HB3  | 1:120:B:ILE:HB    | 11       | 0.12          |
| (2,470)  | 1:125:B:SER:H    | 1:124:B:ILE:HG21  | 8        | 0.12          |
| (2,448)  | 1:131:B:ASN:H    | 1:131:B:ASN:HD21  | 1        | 0.12          |
| (2,394)  | 1:117:B:ASP:H    | 1:116:B:MET:HB2   | 4        | 0.12          |
| (2,387)  | 1:116:B:MET:H    | 1:115:B:GLN:HB2   | 4        | 0.12          |
| (2,351)  | 1:133:B:GLU:H    | 1:133:B:GLU:HG3   | 19       | 0.12          |
| (2,247)  | 2:1781:A:ILE:H   | 2:1779:A:CYS:HB2  | 4        | 0.12          |
| (2,247)  | 2:1781:A:ILE:H   | 2:1779:A:CYS:HB2  | 14       | 0.12          |
| (2,247)  | 2:1781:A:ILE:H   | 2:1779:A:CYS:HB2  | 17       | 0.12          |
| (2,212)  | 2:1740:A:GLN:H   | 2:1743:A:VAL:HG13 | 13       | 0.12          |
| (2,114)  | 2:1760:A:LYS:HG3 | 2:1760:A:LYS:H    | 7        | 0.12          |
| (2,108)  | 2:1741:A:SER:H   | 2:1761:A:MET:HE1  | 1        | 0.12          |
| (2,108)  | 2:1741:A:SER:H   | 2:1761:A:MET:HE2  | 3        | 0.12          |
| (2,108)  | 2:1741:A:SER:H   | 2:1761:A:MET:HE1  | 13       | 0.12          |
| (1,35)   | 2:1808:A:ASN:H   | 2:1804:A:PRO:O    | 3        | 0.12          |
| (3,36)   | 2:1745:A:ALA:HB2 | 2:1761:A:MET:HG3  | 19       | 0.11          |
| (3,30)   | 2:1794:A:LYS:HG3 | 2:1794:A:LYS:HB2  | 6        | 0.11          |
| (3,30)   | 2:1794:A:LYS:HG3 | 2:1794:A:LYS:HB2  | 12       | 0.11          |
| (3,30)   | 2:1794:A:LYS:HG3 | 2:1794:A:LYS:HB2  | 13       | 0.11          |
| (3,30)   | 2:1794:A:LYS:HG3 | 2:1794:A:LYS:HD2  | 15       | 0.11          |
| (3,30)   | 2:1794:A:LYS:HG3 | 2:1794:A:LYS:HB2  | 20       | 0.11          |
| (2,1733) | 2:1758:A:CYS:HB3 | 2:1744:A:HIS:HD2  | 10       | 0.11          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 1        | 0.11          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 9        | 0.11          |
| (2,1726) | 2:1767:A:HIS:HD2  | 2:1768:A:THR:HA   | 19       | 0.11          |
| (2,1707) | 2:1748:A:CYS:HB3  | 2:1747:A:GLN:H    | 20       | 0.11          |
| (2,1685) | 2:1747:A:GLN:HG3  | 2:1743:A:VAL:HG21 | 11       | 0.11          |
| (2,1631) | 2:1809:A:ILE:HG12 | 2:1793:A:ALA:HB3  | 3        | 0.11          |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 1        | 0.11          |
| (2,1562) | 2:1768:A:THR:HB   | 2:1767:A:HIS:HD2  | 5        | 0.11          |
| (2,1530) | 2:1746:A:ALA:HB1  | 2:1802:A:PRO:HB2  | 3        | 0.11          |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 18       | 0.11          |
| (2,1519) | 2:1756:A:PRO:HD3  | 2:1755:A:LEU:HA   | 17       | 0.11          |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 7        | 0.11          |
| (2,1506) | 2:1781:A:ILE:HD13 | 2:1781:A:ILE:H    | 15       | 0.11          |
| (2,1493) | 2:1769:A:LYS:HE3  | 2:1769:A:LYS:HG2  | 16       | 0.11          |
| (2,1451) | 2:1789:A:ALA:HB3  | 2:1805:A:PHE:HD2  | 18       | 0.11          |
| (2,1438) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:H    | 14       | 0.11          |
| (2,1406) | 2:1763:A:ARG:HA   | 2:1763:A:ARG:HG2  | 13       | 0.11          |
| (2,1371) | 2:1764:A:VAL:HG23 | 2:1764:A:VAL:H    | 6        | 0.11          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 5        | 0.11          |
| (2,1356) | 2:1725:A:GLN:HB2  | 2:1725:A:GLN:HG2  | 13       | 0.11          |
| (2,1355) | 2:1780:A:PRO:HD3  | 2:1781:A:ILE:H    | 1        | 0.11          |
| (2,1336) | 2:1772:A:LYS:HA   | 2:1772:A:LYS:HD3  | 18       | 0.11          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB3  | 2        | 0.11          |
| (2,1303) | 2:1751:A:ALA:HA   | 2:1751:A:ALA:HB3  | 19       | 0.11          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 6        | 0.11          |
| (2,1280) | 2:1784:A:GLN:HG2  | 2:1784:A:GLN:HE22 | 20       | 0.11          |
| (2,1274) | 2:1759:A:GLN:HG3  | 2:1760:A:LYS:H    | 7        | 0.11          |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 4        | 0.11          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 11       | 0.11          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 14       | 0.11          |
| (2,1232) | 2:1784:A:GLN:HB3  | 2:1784:A:GLN:H    | 16       | 0.11          |
| (2,1200) | 2:1762:A:LYS:HG3  | 2:1762:A:LYS:H    | 6        | 0.11          |
| (2,1169) | 2:1741:A:SER:HA   | 2:1744:A:HIS:H    | 11       | 0.11          |
| (2,1135) | 2:1765:A:VAL:HG13 | 2:1804:A:PRO:HG2  | 12       | 0.11          |
| (2,1127) | 2:1761:A:MET:HE2  | 2:1738:A:ALA:HB3  | 16       | 0.11          |
| (2,1116) | 2:1747:A:GLN:HG2  | 2:1747:A:GLN:HE22 | 18       | 0.11          |
| (2,1099) | 2:1783:A:LYS:HE2  | 2:1783:A:LYS:HD3  | 10       | 0.11          |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 12       | 0.11          |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 10       | 0.11          |
| (2,1023) | 2:1779:A:CYS:HB2  | 2:1774:A:LYS:HD3  | 14       | 0.11          |
| (2,1014) | 2:1733:A:LEU:HD21 | 2:1733:A:LEU:H    | 15       | 0.11          |
| (2,1004) | 2:1738:A:ALA:HB1  | 2:1738:A:ALA:H    | 16       | 0.11          |

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| Key     | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|---------|------------------|-------------------|----------|---------------|
| (2,979) | 2:1757:A:SER:HA  | 2:1760:A:LYS:HB2  | 6        | 0.11          |
| (2,953) | 2:1780:A:PRO:HB3 | 2:1781:A:ILE:H    | 13       | 0.11          |
| (2,953) | 2:1780:A:PRO:HB3 | 2:1781:A:ILE:H    | 17       | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 4        | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 5        | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 6        | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 12       | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 15       | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 18       | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 19       | 0.11          |
| (2,917) | 2:1763:A:ARG:HG3 | 2:1763:A:ARG:H    | 20       | 0.11          |
| (2,914) | 2:1760:A:LYS:HG2 | 2:1760:A:LYS:HB2  | 1        | 0.11          |
| (2,914) | 2:1760:A:LYS:HG2 | 2:1760:A:LYS:HB2  | 7        | 0.11          |
| (2,914) | 2:1760:A:LYS:HG2 | 2:1760:A:LYS:HB2  | 16       | 0.11          |
| (2,906) | 2:1759:A:GLN:HB2 | 2:1759:A:GLN:HA   | 7        | 0.11          |
| (2,906) | 2:1759:A:GLN:HB2 | 2:1759:A:GLN:HA   | 13       | 0.11          |
| (2,906) | 2:1759:A:GLN:HB2 | 2:1759:A:GLN:HA   | 19       | 0.11          |
| (2,882) | 2:1807:A:LEU:HG  | 2:1807:A:LEU:H    | 4        | 0.11          |
| (2,882) | 2:1807:A:LEU:HG  | 2:1807:A:LEU:H    | 9        | 0.11          |
| (2,867) | 2:1785:A:LEU:HG  | 2:1785:A:LEU:H    | 11       | 0.11          |
| (2,867) | 2:1785:A:LEU:HG  | 2:1785:A:LEU:H    | 12       | 0.11          |
| (2,846) | 2:1742:A:LEU:HA  | 2:1745:A:ALA:HB2  | 19       | 0.11          |
| (2,786) | 2:1805:A:PHE:HB2 | 2:1809:A:ILE:HD11 | 5        | 0.11          |
| (2,757) | 2:1783:A:LYS:HE2 | 2:1783:A:LYS:H    | 6        | 0.11          |
| (2,723) | 2:1804:A:PRO:HA  | 2:1806:A:CYS:H    | 8        | 0.11          |
| (2,723) | 2:1804:A:PRO:HA  | 2:1806:A:CYS:H    | 11       | 0.11          |
| (2,723) | 2:1804:A:PRO:HA  | 2:1806:A:CYS:H    | 17       | 0.11          |
| (2,718) | 2:1787:A:ALA:HB2 | 2:1787:A:ALA:H    | 5        | 0.11          |
| (2,718) | 2:1787:A:ALA:HB2 | 2:1787:A:ALA:H    | 12       | 0.11          |
| (2,717) | 2:1790:A:ALA:HB1 | 2:1790:A:ALA:H    | 16       | 0.11          |
| (2,657) | 1:135:B:LEU:HD22 | 1:130:B:TYR:HD2   | 4        | 0.11          |
| (2,647) | 1:133:B:GLU:HB3  | 1:131:B:ASN:HD22  | 6        | 0.11          |
| (2,645) | 1:132:B:GLU:HB2  | 1:130:B:TYR:HE1   | 10       | 0.11          |
| (2,638) | 1:115:B:GLN:HG2  | 1:115:B:GLN:HA    | 7        | 0.11          |
| (2,598) | 1:116:B:MET:HA   | 1:116:B:MET:HG3   | 5        | 0.11          |
| (2,598) | 1:116:B:MET:HA   | 1:116:B:MET:HG3   | 19       | 0.11          |
| (2,576) | 1:119:B:VAL:HG12 | 1:120:B:ILE:H     | 9        | 0.11          |
| (2,576) | 1:119:B:VAL:HG11 | 1:120:B:ILE:H     | 10       | 0.11          |
| (2,576) | 1:119:B:VAL:HG13 | 1:120:B:ILE:H     | 12       | 0.11          |
| (2,576) | 1:119:B:VAL:HG13 | 1:120:B:ILE:H     | 13       | 0.11          |
| (2,557) | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD12  | 2        | 0.11          |
| (2,557) | 1:124:B:ILE:HG13 | 1:124:B:ILE:HD11  | 3        | 0.11          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (2,557) | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD12  | 4        | 0.11          |
| (2,557) | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD12  | 5        | 0.11          |
| (2,557) | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD12  | 6        | 0.11          |
| (2,557) | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD11  | 9        | 0.11          |
| (2,557) | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD11  | 12       | 0.11          |
| (2,557) | 1:124:B:ILE:HG13  | 1:124:B:ILE:HD12  | 16       | 0.11          |
| (2,510) | 1:117:B:ASP:HA    | 1:119:B:VAL:HG21  | 13       | 0.11          |
| (2,509) | 1:117:B:ASP:HA    | 1:117:B:ASP:HB3   | 7        | 0.11          |
| (2,509) | 1:117:B:ASP:HA    | 1:117:B:ASP:HB3   | 12       | 0.11          |
| (2,501) | 1:120:B:ILE:HG12  | 1:120:B:ILE:HA    | 7        | 0.11          |
| (2,501) | 1:120:B:ILE:HG12  | 1:120:B:ILE:HA    | 9        | 0.11          |
| (2,501) | 1:120:B:ILE:HG12  | 1:120:B:ILE:HA    | 12       | 0.11          |
| (2,501) | 1:120:B:ILE:HG12  | 1:120:B:ILE:HA    | 15       | 0.11          |
| (2,487) | 1:117:B:ASP:HB3   | 1:120:B:ILE:HB    | 6        | 0.11          |
| (2,483) | 1:126:B:LEU:HD23  | 1:127:B:GLU:H     | 20       | 0.11          |
| (2,472) | 1:123:B:ILE:H     | 1:123:B:ILE:HD11  | 4        | 0.11          |
| (2,472) | 1:123:B:ILE:H     | 1:123:B:ILE:HD12  | 10       | 0.11          |
| (2,472) | 1:123:B:ILE:H     | 1:123:B:ILE:HD11  | 20       | 0.11          |
| (2,455) | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 2        | 0.11          |
| (2,455) | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 6        | 0.11          |
| (2,455) | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 9        | 0.11          |
| (2,455) | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 13       | 0.11          |
| (2,455) | 1:136:B:GLY:H     | 1:132:B:GLU:HG2   | 19       | 0.11          |
| (2,398) | 1:139:B:ASP:H     | 1:138:B:MET:HB2   | 8        | 0.11          |
| (2,386) | 1:126:B:LEU:H     | 1:126:B:LEU:HD11  | 3        | 0.11          |
| (2,351) | 1:133:B:GLU:H     | 1:133:B:GLU:HG3   | 3        | 0.11          |
| (2,340) | 1:130:B:TYR:H     | 1:130:B:TYR:HD1   | 2        | 0.11          |
| (2,340) | 1:130:B:TYR:H     | 1:130:B:TYR:HD2   | 8        | 0.11          |
| (2,338) | 1:124:B:ILE:H     | 1:124:B:ILE:HG12  | 8        | 0.11          |
| (2,291) | 2:1750:A:ASN:HD22 | 2:1752:A:ASN:HB3  | 18       | 0.11          |
| (2,290) | 2:1773:A:ARG:H    | 2:1773:A:ARG:HG2  | 19       | 0.11          |
| (2,277) | 2:1738:A:ALA:H    | 2:1737:A:ARG:HD2  | 9        | 0.11          |
| (2,247) | 2:1781:A:ILE:H    | 2:1779:A:CYS:HB2  | 16       | 0.11          |
| (2,212) | 2:1740:A:GLN:H    | 2:1743:A:VAL:HG11 | 4        | 0.11          |
| (2,212) | 2:1740:A:GLN:H    | 2:1743:A:VAL:HG13 | 19       | 0.11          |
| (2,197) | 2:1761:A:MET:H    | 2:1759:A:GLN:H    | 11       | 0.11          |
| (2,197) | 2:1761:A:MET:H    | 2:1759:A:GLN:H    | 20       | 0.11          |
| (2,193) | 2:1809:A:ILE:HG12 | 2:1809:A:ILE:H    | 11       | 0.11          |
| (2,130) | 2:1731:A:ARG:H    | 2:1731:A:ARG:HB2  | 3        | 0.11          |
| (2,108) | 2:1741:A:SER:H    | 2:1761:A:MET:HE2  | 5        | 0.11          |
| (1,35)  | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 6        | 0.11          |
| (1,35)  | 2:1808:A:ASN:H    | 2:1804:A:PRO:O    | 19       | 0.11          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (3,36)   | 2:1745:A:ALA:HB3  | 2:1761:A:MET:HG3  | 12       | 0.1           |
| (3,30)   | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HB2  | 2        | 0.1           |
| (3,30)   | 2:1794:A:LYS:HG3  | 2:1794:A:LYS:HB2  | 18       | 0.1           |
| (3,9)    | 1:120:B:ILE:HG21  | 1:120:B:ILE:HG12  | 3        | 0.1           |
| (2,1716) | 2:1785:A:LEU:HB2  | 2:1805:A:PHE:HE2  | 3        | 0.1           |
| (2,1698) | 2:1788:A:LEU:HD23 | 2:1787:A:ALA:H    | 20       | 0.1           |
| (2,1637) | 2:1810:A:LYS:HD2  | 2:1810:A:LYS:H    | 2        | 0.1           |
| (2,1623) | 2:1747:A:GLN:HB2  | 2:1747:A:GLN:HE22 | 3        | 0.1           |
| (2,1616) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HG2  | 19       | 0.1           |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 2        | 0.1           |
| (2,1581) | 2:1804:A:PRO:HB3  | 2:1765:A:VAL:HA   | 5        | 0.1           |
| (2,1534) | 2:1781:A:ILE:HG12 | 2:1781:A:ILE:H    | 19       | 0.1           |
| (2,1520) | 2:1756:A:PRO:HD2  | 2:1755:A:LEU:HA   | 19       | 0.1           |
| (2,1506) | 2:1781:A:ILE:HD11 | 2:1781:A:ILE:H    | 5        | 0.1           |
| (2,1474) | 2:1790:A:ALA:HA   | 2:1809:A:ILE:HD12 | 2        | 0.1           |
| (2,1438) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:H    | 6        | 0.1           |
| (2,1438) | 2:1788:A:LEU:HB3  | 2:1788:A:LEU:H    | 19       | 0.1           |
| (2,1371) | 2:1764:A:VAL:HG23 | 2:1764:A:VAL:H    | 4        | 0.1           |
| (2,1300) | 2:1761:A:MET:HA   | 2:1765:A:VAL:H    | 17       | 0.1           |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 7        | 0.1           |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 15       | 0.1           |
| (2,1234) | 2:1796:A:CYS:HB3  | 2:1793:A:ALA:HA   | 17       | 0.1           |
| (2,1179) | 2:1755:A:LEU:HD13 | 2:1755:A:LEU:H    | 5        | 0.1           |
| (2,1163) | 2:1758:A:CYS:HA   | 2:1744:A:HIS:HD2  | 10       | 0.1           |
| (2,1131) | 2:1761:A:MET:HE1  | 2:1742:A:LEU:H    | 2        | 0.1           |
| (2,1110) | 2:1747:A:GLN:HB2  | 2:1747:A:GLN:H    | 8        | 0.1           |
| (2,1110) | 2:1747:A:GLN:HB2  | 2:1747:A:GLN:H    | 18       | 0.1           |
| (2,1051) | 2:1780:A:PRO:HA   | 2:1783:A:LYS:HB3  | 20       | 0.1           |
| (2,1031) | 2:1740:A:GLN:HB3  | 2:1741:A:SER:H    | 8        | 0.1           |
| (2,1014) | 2:1733:A:LEU:HD22 | 2:1733:A:LEU:H    | 11       | 0.1           |
| (2,1006) | 2:1781:A:ILE:HA   | 2:1784:A:GLN:HB3  | 13       | 0.1           |
| (2,1004) | 2:1738:A:ALA:HB2  | 2:1738:A:ALA:H    | 4        | 0.1           |
| (2,1004) | 2:1738:A:ALA:HB2  | 2:1738:A:ALA:H    | 10       | 0.1           |
| (2,998)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HG3  | 15       | 0.1           |
| (2,998)  | 2:1811:A:GLN:HA   | 2:1811:A:GLN:HG3  | 20       | 0.1           |
| (2,979)  | 2:1757:A:SER:HA   | 2:1760:A:LYS:HB2  | 17       | 0.1           |
| (2,964)  | 2:1739:A:ILE:HB   | 2:1739:A:ILE:HD13 | 4        | 0.1           |
| (2,953)  | 2:1780:A:PRO:HB3  | 2:1781:A:ILE:H    | 20       | 0.1           |
| (2,948)  | 2:1760:A:LYS:HB2  | 2:1760:A:LYS:HE2  | 6        | 0.1           |
| (2,923)  | 2:1765:A:VAL:HG23 | 2:1745:A:ALA:HB1  | 6        | 0.1           |
| (2,917)  | 2:1763:A:ARG:HG3  | 2:1763:A:ARG:H    | 3        | 0.1           |
| (2,906)  | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA   | 2        | 0.1           |

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| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (2,906) | 2:1759:A:GLN:HB2  | 2:1759:A:GLN:HA  | 16       | 0.1           |
| (2,903) | 2:1768:A:THR:HA   | 2:1771:A:CYS:H   | 20       | 0.1           |
| (2,882) | 2:1807:A:LEU:HG   | 2:1807:A:LEU:H   | 7        | 0.1           |
| (2,868) | 2:1727:A:PRO:HD3  | 2:1727:A:PRO:HG2 | 19       | 0.1           |
| (2,867) | 2:1785:A:LEU:HG   | 2:1785:A:LEU:H   | 3        | 0.1           |
| (2,846) | 2:1742:A:LEU:HA   | 2:1745:A:ALA:HB1 | 6        | 0.1           |
| (2,826) | 2:1791:A:TYR:HA   | 2:1794:A:LYS:HB2 | 3        | 0.1           |
| (2,826) | 2:1791:A:TYR:HA   | 2:1794:A:LYS:HB2 | 5        | 0.1           |
| (2,718) | 2:1787:A:ALA:HB3  | 2:1787:A:ALA:H   | 10       | 0.1           |
| (2,526) | 1:132:B:GLU:HG2   | 1:132:B:GLU:HA   | 5        | 0.1           |
| (2,511) | 1:119:B:VAL:H     | 1:118:B:ASP:HA   | 18       | 0.1           |
| (2,509) | 1:117:B:ASP:HA    | 1:117:B:ASP:HB3  | 15       | 0.1           |
| (2,501) | 1:120:B:ILE:HG12  | 1:120:B:ILE:HA   | 8        | 0.1           |
| (2,500) | 1:135:B:LEU:HG    | 1:135:B:LEU:H    | 7        | 0.1           |
| (2,483) | 1:126:B:LEU:HD21  | 1:127:B:GLU:H    | 7        | 0.1           |
| (2,483) | 1:126:B:LEU:HD22  | 1:127:B:GLU:H    | 11       | 0.1           |
| (2,472) | 1:123:B:ILE:H     | 1:123:B:ILE:HD12 | 5        | 0.1           |
| (2,472) | 1:123:B:ILE:H     | 1:123:B:ILE:HD11 | 7        | 0.1           |
| (2,444) | 1:120:B:ILE:H     | 1:120:B:ILE:HB   | 1        | 0.1           |
| (2,394) | 1:117:B:ASP:H     | 1:116:B:MET:HB2  | 8        | 0.1           |
| (2,366) | 1:137:B:LEU:H     | 1:135:B:LEU:HA   | 20       | 0.1           |
| (2,340) | 1:130:B:TYR:H     | 1:130:B:TYR:HD1  | 17       | 0.1           |
| (2,338) | 1:124:B:ILE:H     | 1:124:B:ILE:HG12 | 2        | 0.1           |
| (2,321) | 2:1777:A:GLY:H    | 2:1776:A:ASN:HA  | 8        | 0.1           |
| (2,279) | 2:1742:A:LEU:H    | 2:1743:A:VAL:HA  | 4        | 0.1           |
| (2,192) | 2:1784:A:GLN:HE22 | 1:134:B:ILE:HG21 | 20       | 0.1           |
| (2,114) | 2:1760:A:LYS:HG3  | 2:1760:A:LYS:H   | 15       | 0.1           |
| (2,108) | 2:1741:A:SER:H    | 2:1761:A:MET:HE1 | 2        | 0.1           |
| (2,108) | 2:1741:A:SER:H    | 2:1761:A:MET:HE1 | 16       | 0.1           |
| (2,108) | 2:1741:A:SER:H    | 2:1761:A:MET:HE3 | 18       | 0.1           |

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

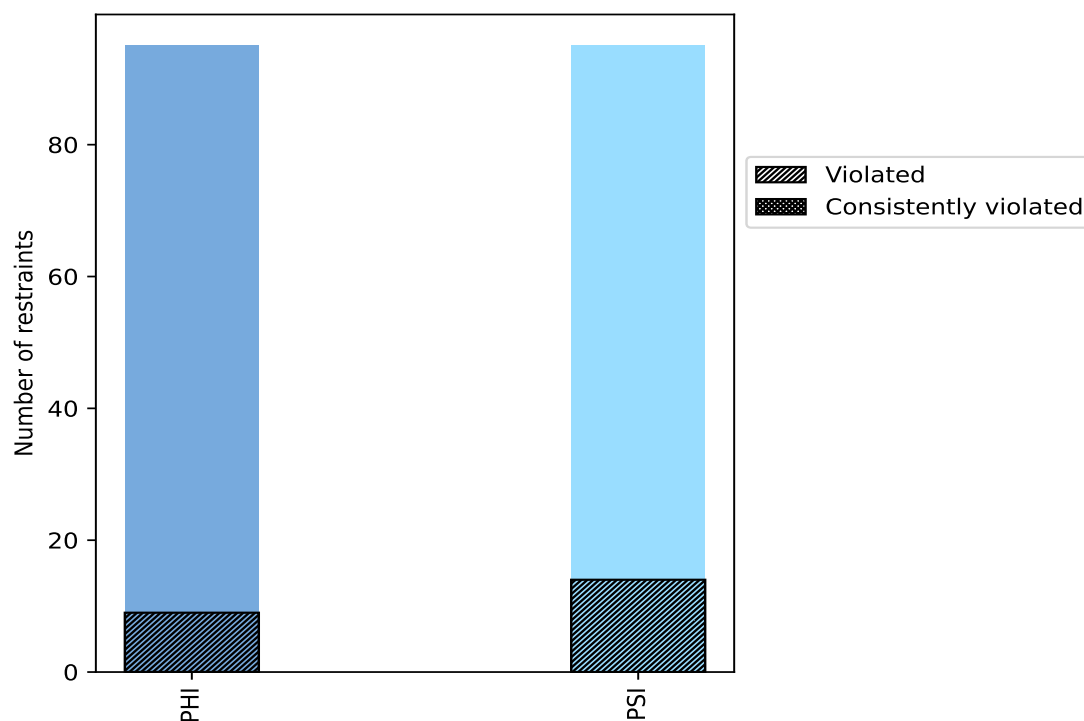
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 95    | 50.0           | 9                     | 9.5            | 4.7            | 0                                  | 0.0            | 0.0            |
| PSI        | 95    | 50.0           | 14                    | 14.7           | 7.4            | 0                                  | 0.0            | 0.0            |
| Total      | 190   | 100.0          | 23                    | 12.1           | 12.1           | 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](#)



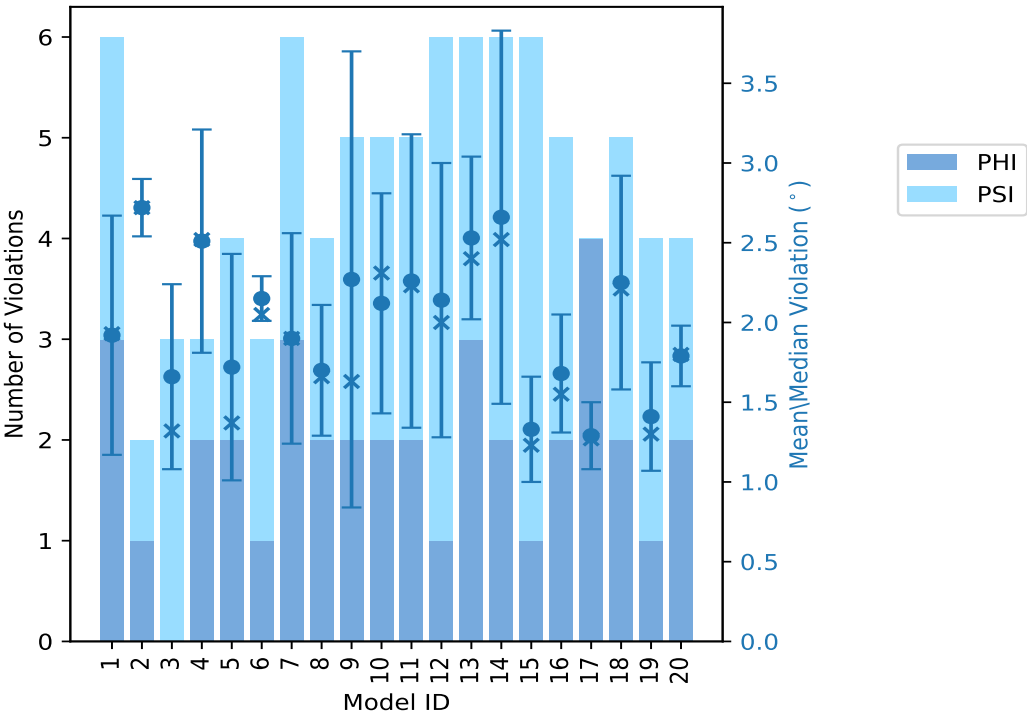
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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        | 3                    | 3   | 6     | 1.92     | 2.87    | 0.75   | 1.93       |
| 2        | 1                    | 1   | 2     | 2.72     | 2.9     | 0.18   | 2.72       |
| 3        | 0                    | 3   | 3     | 1.66     | 2.47    | 0.58   | 1.32       |
| 4        | 2                    | 1   | 3     | 2.51     | 3.36    | 0.7    | 2.52       |
| 5        | 2                    | 2   | 4     | 1.72     | 2.93    | 0.71   | 1.37       |
| 6        | 1                    | 2   | 3     | 2.15     | 2.35    | 0.14   | 2.05       |
| 7        | 3                    | 3   | 6     | 1.9      | 2.72    | 0.66   | 1.9        |
| 8        | 2                    | 2   | 4     | 1.7      | 2.19    | 0.41   | 1.66       |
| 9        | 2                    | 3   | 5     | 2.27     | 5.05    | 1.43   | 1.63       |
| 10       | 2                    | 3   | 5     | 2.12     | 3.01    | 0.69   | 2.31       |
| 11       | 2                    | 3   | 5     | 2.26     | 3.74    | 0.92   | 2.23       |
| 12       | 1                    | 5   | 6     | 2.14     | 3.86    | 0.86   | 2.0        |
| 13       | 3                    | 3   | 6     | 2.53     | 3.51    | 0.51   | 2.4        |
| 14       | 2                    | 4   | 6     | 2.66     | 4.96    | 1.17   | 2.52       |
| 15       | 1                    | 5   | 6     | 1.33     | 2.06    | 0.33   | 1.23       |
| 16       | 2                    | 3   | 5     | 1.68     | 2.22    | 0.37   | 1.55       |
| 17       | 4                    | 0   | 4     | 1.29     | 1.61    | 0.21   | 1.27       |
| 18       | 2                    | 3   | 5     | 2.25     | 3.42    | 0.67   | 2.21       |
| 19       | 1                    | 3   | 4     | 1.41     | 1.95    | 0.34   | 1.3        |
| 20       | 2                    | 2   | 4     | 1.79     | 2.03    | 0.19   | 1.8        |

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>       | %    |
| 6                             | 5   | 11    | 1                        | 5.0  |
| 1                             | 4   | 5     | 2                        | 10.0 |
| 0                             | 0   | 0     | 3                        | 15.0 |
| 0                             | 1   | 1     | 4                        | 20.0 |
| 0                             | 0   | 0     | 5                        | 25.0 |
| 0                             | 1   | 1     | 6                        | 30.0 |
| 0                             | 0   | 0     | 7                        | 35.0 |
| 0                             | 1   | 1     | 8                        | 40.0 |
| 0                             | 1   | 1     | 9                        | 45.0 |
| 0                             | 0   | 0     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

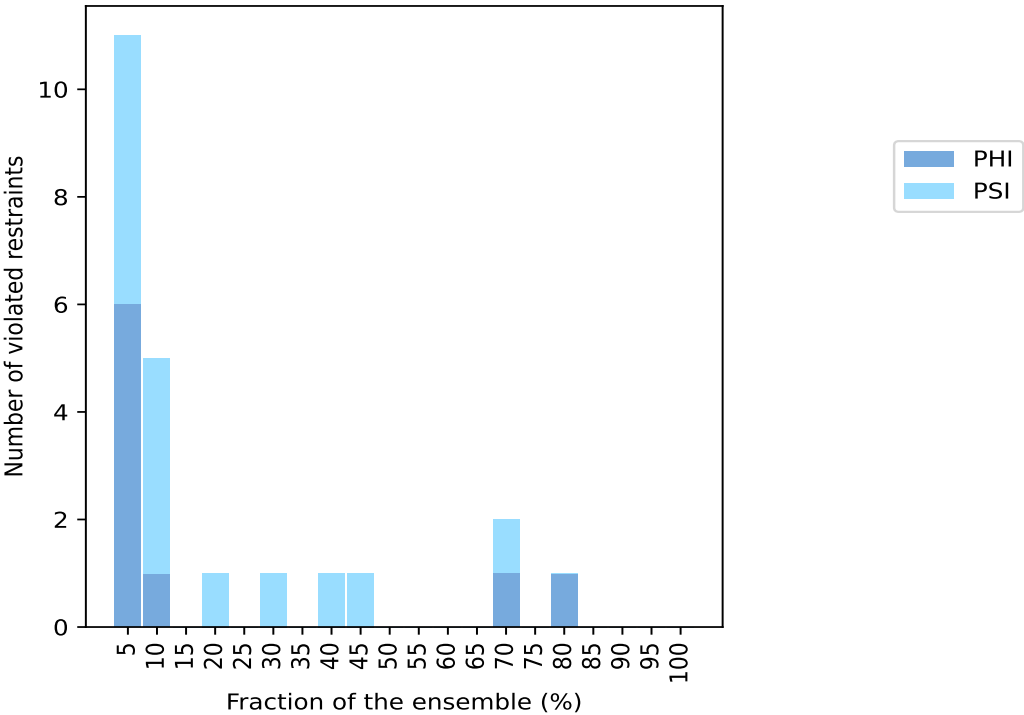
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 1                             | 1   | 2     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 1                             | 0   | 1     | 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 ⓘ

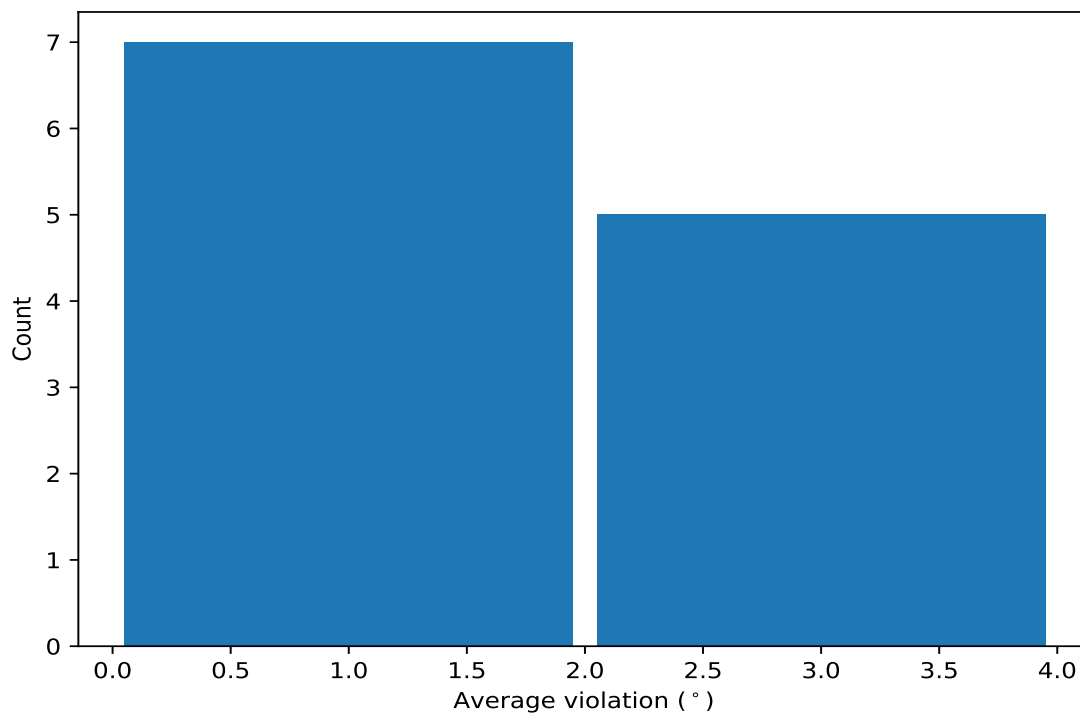


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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.

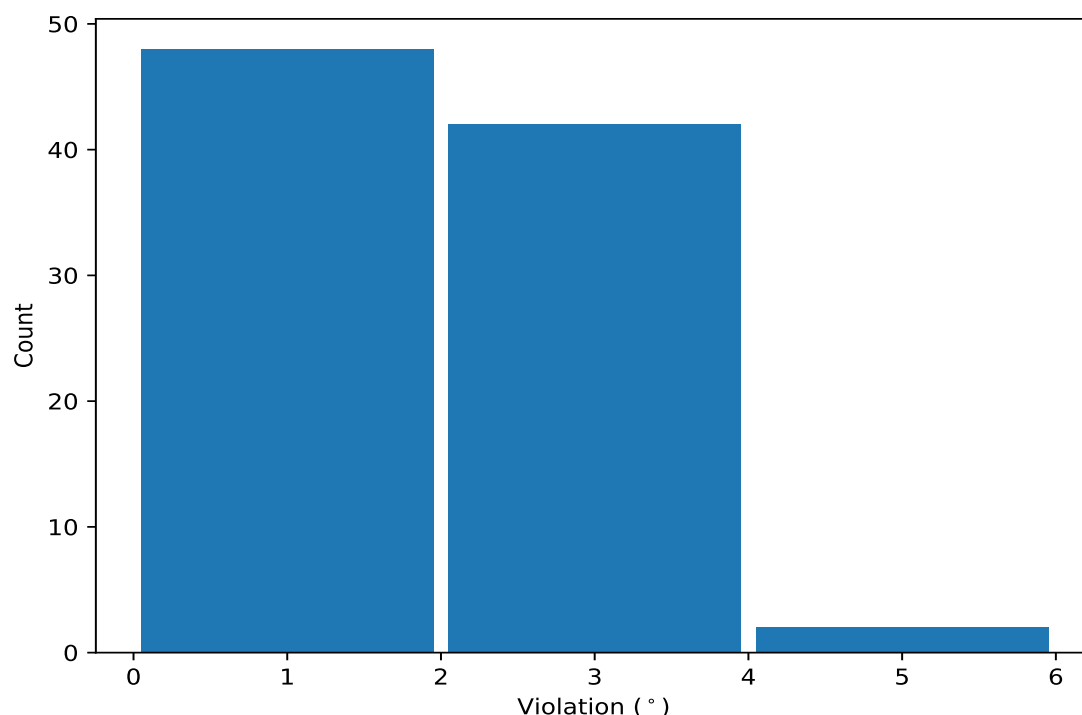
| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Medi |
|---------|----------------|-----------------|-----------------|----------------|---------------------|------|-----------------|------|
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 16                  | 2.03 | 0.91            | 1.94 |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 14                  | 2.56 | 1.03            | 2.42 |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 14                  | 2.26 | 0.44            | 2.19 |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 9                   | 1.61 | 0.58            | 1.29 |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 8                   | 2.02 | 0.57            | 2.14 |
| (1,92)  | 2:1779:A:CYS:N | 2:1779:A:CYS:CA | 2:1779:A:CYS:C  | 2:1780:A:PRO:N | 6                   | 1.99 | 0.91            | 1.62 |
| (1,184) | 1:135:B:LEU:N  | 1:135:B:LEU:CA  | 1:135:B:LEU:C   | 1:136:B:GLY:N  | 4                   | 1.95 | 0.71            | 1.93 |
| (1,83)  | 2:1773:A:ARG:C | 2:1774:A:LYS:N  | 2:1774:A:LYS:CA | 2:1774:A:LYS:C | 2                   | 2.19 | 0.51            | 2.19 |
| (1,2)   | 2:1723:A:ALA:N | 2:1723:A:ALA:CA | 2:1723:A:ALA:C  | 2:1724:A:THR:N | 2                   | 1.92 | 0.02            | 1.92 |
| (1,80)  | 2:1768:A:THR:N | 2:1768:A:THR:CA | 2:1768:A:THR:C  | 2:1769:A:LYS:N | 2                   | 1.66 | 0.55            | 1.66 |
| (1,88)  | 2:1776:A:ASN:N | 2:1776:A:ASN:CA | 2:1776:A:ASN:C  | 2:1777:A:GLY:N | 2                   | 1.31 | 0.22            | 1.31 |
| (1,4)   | 2:1725:A:GLN:N | 2:1725:A:GLN:CA | 2:1725:A:GLN:C  | 2:1726:A:SER:N | 2                   | 1.18 | 0.08            | 1.18 |

<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 (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 9        | 5.05          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 14       | 4.96          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 12       | 3.86          |
| (1,92)  | 2:1779:A:CYS:N | 2:1779:A:CYS:CA | 2:1779:A:CYS:C  | 2:1780:A:PRO:N | 11       | 3.74          |
| (1,123) | 2:1794:A:LYS:C | 2:1795:A:HIS:N  | 2:1795:A:HIS:CA | 2:1795:A:HIS:C | 13       | 3.51          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 18       | 3.42          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 4        | 3.36          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 10       | 3.01          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 5        | 2.93          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 2        | 2.9           |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 1        | 2.87          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 14       | 2.79          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 13       | 2.77          |
| (1,184) | 1:135:B:LEU:N  | 1:135:B:LEU:CA  | 1:135:B:LEU:C   | 1:136:B:GLY:N  | 1        | 2.72          |

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| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 7        | 2.72          |
| (1,83)  | 2:1773:A:ARG:C | 2:1774:A:LYS:N  | 2:1774:A:LYS:CA | 2:1774:A:LYS:C | 7        | 2.7           |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 11       | 2.65          |
| (1,184) | 1:135:B:LEU:N  | 1:135:B:LEU:CA  | 1:135:B:LEU:C   | 1:136:B:GLY:N  | 14       | 2.6           |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 10       | 2.54          |
| (1,92)  | 2:1779:A:CYS:N | 2:1779:A:CYS:CA | 2:1779:A:CYS:C  | 2:1780:A:PRO:N | 2        | 2.54          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 4        | 2.52          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 13       | 2.5           |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 3        | 2.47          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 14       | 2.43          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 18       | 2.37          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 6        | 2.35          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 10       | 2.31          |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 12       | 2.3           |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 13       | 2.29          |
| (1,187) | 1:137:B:LEU:C  | 1:138:B:MET:N   | 1:138:B:MET:CA  | 1:138:B:MET:C  | 1        | 2.28          |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 13       | 2.25          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 11       | 2.23          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 16       | 2.22          |
| (1,80)  | 2:1768:A:THR:N | 2:1768:A:THR:CA | 2:1768:A:THR:C  | 2:1769:A:LYS:N | 18       | 2.21          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 8        | 2.19          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 9        | 2.15          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 14       | 2.08          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 12       | 2.06          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 15       | 2.06          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 6        | 2.05          |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 6        | 2.04          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 20       | 2.03          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 16       | 2.02          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 8        | 2.01          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 7        | 1.98          |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 19       | 1.95          |
| (1,2)   | 2:1723:A:ALA:N | 2:1723:A:ALA:CA | 2:1723:A:ALA:C  | 2:1724:A:THR:N | 12       | 1.94          |
| (1,2)   | 2:1723:A:ALA:N | 2:1723:A:ALA:CA | 2:1723:A:ALA:C  | 2:1724:A:THR:N | 20       | 1.91          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 13       | 1.88          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 7        | 1.83          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 18       | 1.81          |
| (1,92)  | 2:1779:A:CYS:N | 2:1779:A:CYS:CA | 2:1779:A:CYS:C  | 2:1780:A:PRO:N | 10       | 1.68          |
| (1,83)  | 2:1773:A:ARG:C | 2:1774:A:LYS:N  | 2:1774:A:LYS:CA | 2:1774:A:LYS:C | 20       | 1.68          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 4        | 1.64          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 9        | 1.63          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 12       | 1.61          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 17       | 1.61          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 11       | 1.59          |
| (1,189) | 1:138:B:MET:C  | 1:139:B:ASP:N   | 1:139:B:ASP:CA  | 1:139:B:ASP:C  | 1        | 1.58          |
| (1,92)  | 2:1779:A:CYS:N | 2:1779:A:CYS:CA | 2:1779:A:CYS:C  | 2:1780:A:PRO:N | 16       | 1.55          |
| (1,88)  | 2:1776:A:ASN:N | 2:1776:A:ASN:CA | 2:1776:A:ASN:C  | 2:1777:A:GLY:N | 20       | 1.53          |
| (1,181) | 1:133:B:GLU:C  | 1:134:B:ILE:N   | 1:134:B:ILE:CA  | 1:134:B:ILE:C  | 5        | 1.49          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 19       | 1.45          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 18       | 1.42          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 16       | 1.37          |

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*Continued from previous page...*

| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,92)  | 2:1779:A:CYS:N | 2:1779:A:CYS:CA | 2:1779:A:CYS:C  | 2:1780:A:PRO:N | 3        | 1.32          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 8        | 1.31          |
| (1,129) | 2:1803:A:VAL:C | 2:1804:A:PRO:N  | 2:1804:A:PRO:CA | 2:1804:A:PRO:C | 17       | 1.3           |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 8        | 1.29          |
| (1,186) | 1:137:B:LEU:N  | 1:137:B:LEU:CA  | 1:137:B:LEU:C   | 1:138:B:MET:N  | 9        | 1.27          |
| (1,184) | 1:135:B:LEU:N  | 1:135:B:LEU:CA  | 1:135:B:LEU:C   | 1:136:B:GLY:N  | 16       | 1.26          |
| (1,4)   | 2:1725:A:GLN:N | 2:1725:A:GLN:CA | 2:1725:A:GLN:C  | 2:1726:A:SER:N | 15       | 1.26          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 5        | 1.25          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 9        | 1.25          |
| (1,93)  | 2:1779:A:CYS:C | 2:1780:A:PRO:N  | 2:1780:A:PRO:CA | 2:1780:A:PRO:C | 17       | 1.25          |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 15       | 1.24          |
| (1,152) | 1:116:B:MET:N  | 1:116:B:MET:CA  | 1:116:B:MET:C   | 1:117:B:ASP:N  | 15       | 1.22          |
| (1,184) | 1:135:B:LEU:N  | 1:135:B:LEU:CA  | 1:135:B:LEU:C   | 1:136:B:GLY:N  | 5        | 1.21          |
| (1,8)   | 2:1727:A:PRO:N | 2:1727:A:PRO:CA | 2:1727:A:PRO:C  | 2:1728:A:GLY:N | 3        | 1.19          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 19       | 1.15          |
| (1,178) | 1:132:B:GLU:N  | 1:132:B:GLU:CA  | 1:132:B:GLU:C   | 1:133:B:GLU:N  | 15       | 1.13          |
| (1,80)  | 2:1768:A:THR:N | 2:1768:A:THR:CA | 2:1768:A:THR:C  | 2:1769:A:LYS:N | 7        | 1.11          |
| (1,88)  | 2:1776:A:ASN:N | 2:1776:A:ASN:CA | 2:1776:A:ASN:C  | 2:1777:A:GLY:N | 19       | 1.09          |
| (1,4)   | 2:1725:A:GLN:N | 2:1725:A:GLN:CA | 2:1725:A:GLN:C  | 2:1726:A:SER:N | 14       | 1.09          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 15       | 1.08          |
| (1,92)  | 2:1779:A:CYS:N | 2:1779:A:CYS:CA | 2:1779:A:CYS:C  | 2:1780:A:PRO:N | 12       | 1.08          |
| (1,130) | 2:1804:A:PRO:N | 2:1804:A:PRO:CA | 2:1804:A:PRO:C  | 2:1805:A:PHE:N | 7        | 1.07          |
| (1,128) | 2:1799:A:ASN:N | 2:1799:A:ASN:CA | 2:1799:A:ASN:C  | 2:1800:A:LYS:N | 11       | 1.07          |
| (1,57)  | 2:1756:A:PRO:C | 2:1757:A:SER:N  | 2:1757:A:SER:CA | 2:1757:A:SER:C | 1        | 1.07          |
| (1,58)  | 2:1757:A:SER:N | 2:1757:A:SER:CA | 2:1757:A:SER:C  | 2:1758:A:CYS:N | 10       | 1.04          |
| (1,132) | 2:1805:A:PHE:N | 2:1805:A:PHE:CA | 2:1805:A:PHE:C  | 2:1806:A:CYS:N | 1        | 1.01          |
| (1,91)  | 2:1778:A:GLY:C | 2:1779:A:CYS:N  | 2:1779:A:CYS:CA | 2:1779:A:CYS:C | 17       | 1.01          |