



# Full wwPDB NMR Structure Validation Report ⓘ

Sep 1, 2026 – 01:18 pm BST

PDB ID : 29JD / pdb\_000029jd  
BMRB ID : 51296  
Title : NMR Structure of the Calcium bound form of OutG, major pilin from *Dickeya dadantii* T2SS  
Authors : Bardiaux, B.; Jacobsen, T.; Dazzoni, R.; Nilges, M.; Francetic, O.; Shevchik, V.; Izadi-Pruneyre, N.  
Deposited on : 2026-03-16

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 : v1.2.1  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

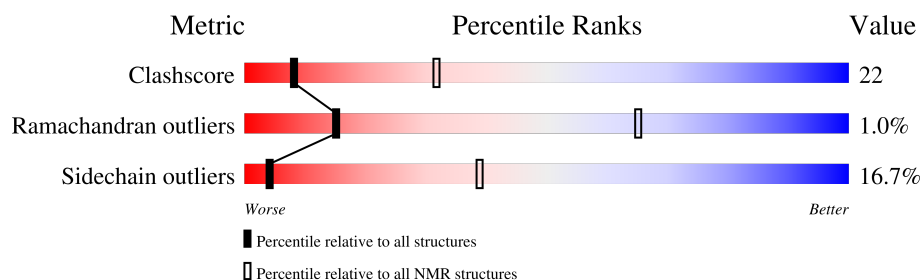
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 85%.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                                                                                                                                                                                                           |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 125    | <div> <div style="width: 43%; background-color: green;"></div> <div style="width: 34%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 16%; background-color: cyan;"></div> </div> <div>43% 34% 6% 16%</div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:28-A:132 (105)      | 0.50              | 1            |

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

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

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

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1854 atoms, of which 901 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Type II secretion system core protein G.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 125      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1853  | 585 | 901 | 169 | 194 | 4 |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 22      | GLY      | -      | expression tag | UNP E0SM38 |
| A     | 23      | MET      | -      | expression tag | UNP E0SM38 |
| A     | 24      | GLY      | -      | expression tag | UNP E0SM38 |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

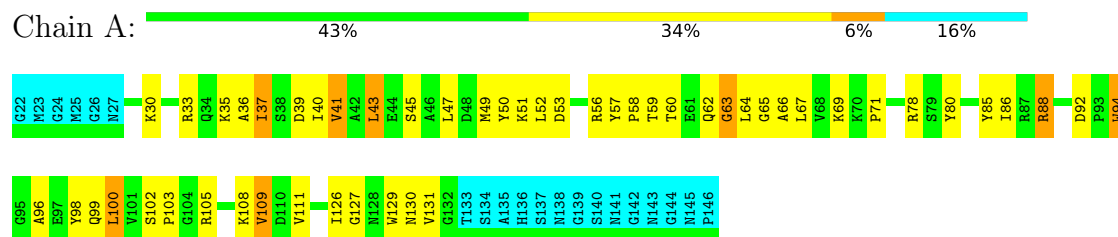
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Ca |
|     |       |          | 1     | 1  |

## 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: Type II secretion system core protein G

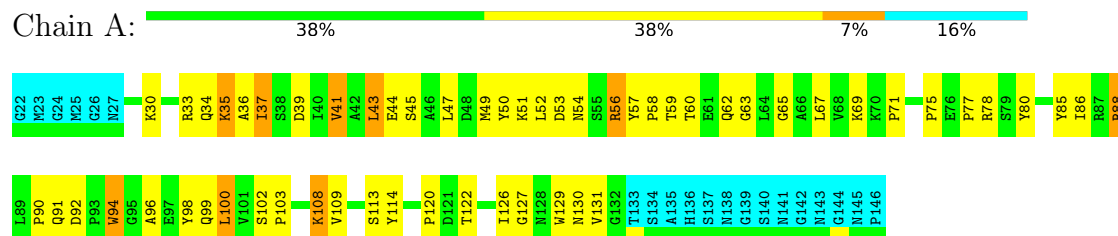


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

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

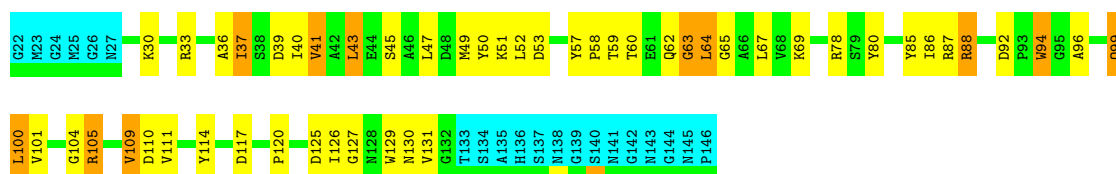
- Molecule 1: Type II secretion system core protein G



#### 4.2.2 Score per residue for model 2

- Molecule 1: Type II secretion system core protein G

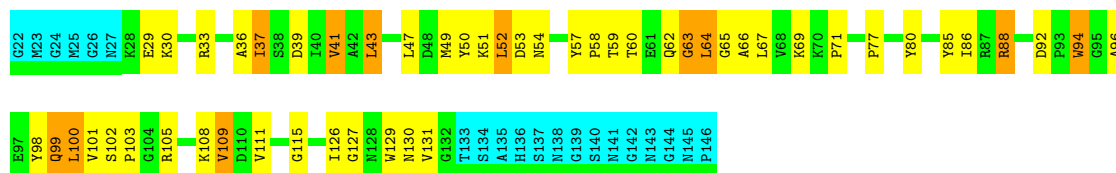




#### 4.2.3 Score per residue for model 3

- Molecule 1: Type II secretion system core protein G

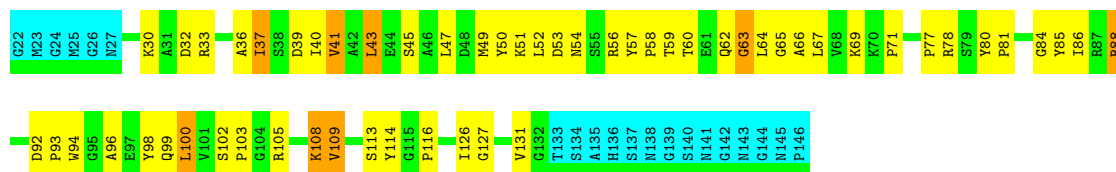
Chain A: 43% 32% 9% 16%



#### 4.2.4 Score per residue for model 4

- Molecule 1: Type II secretion system core protein G

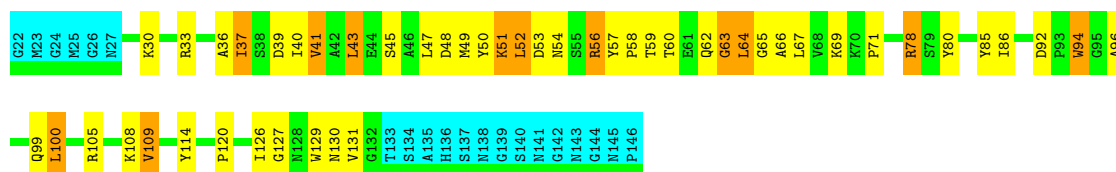
Chain A: 39% 38% 6% 16%



#### 4.2.5 Score per residue for model 5

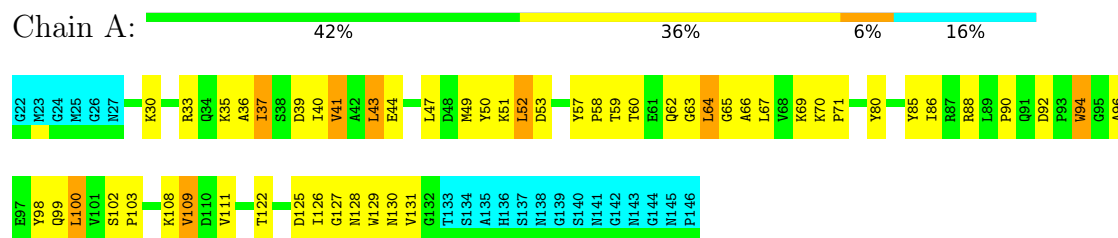
- Molecule 1: Type II secretion system core protein G

Chain A: 45% 30% 10% 16%



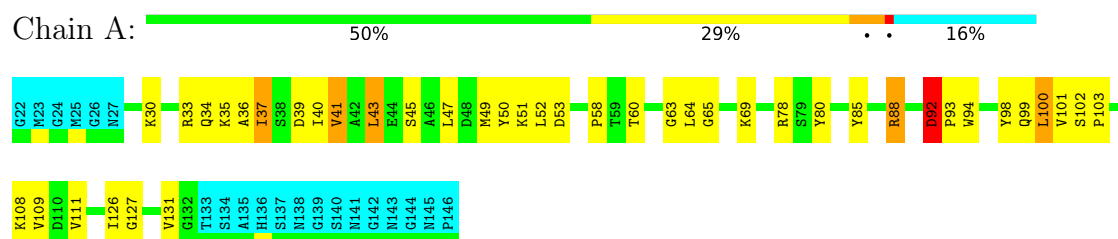
#### 4.2.6 Score per residue for model 6

- Molecule 1: Type II secretion system core protein G



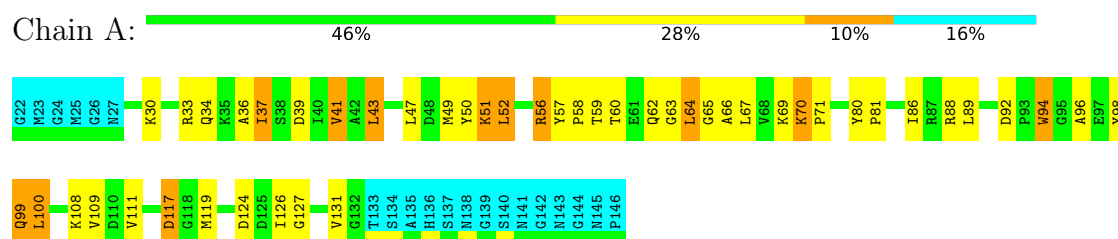
#### 4.2.7 Score per residue for model 7

- Molecule 1: Type II secretion system core protein G



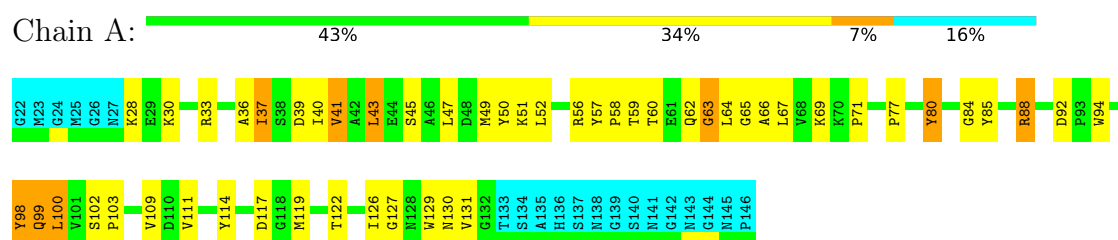
#### 4.2.8 Score per residue for model 8

- Molecule 1: Type II secretion system core protein G



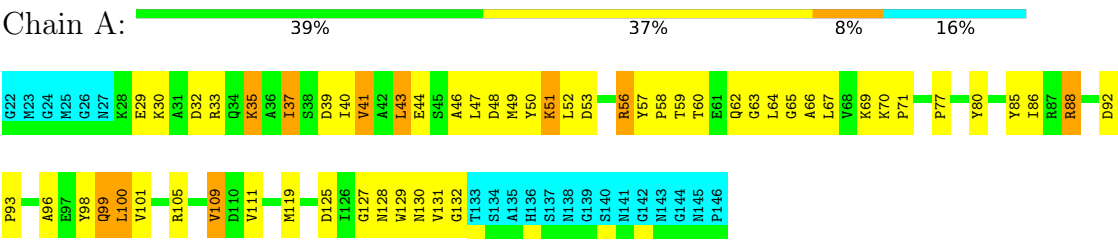
#### 4.2.9 Score per residue for model 9

- Molecule 1: Type II secretion system core protein G



4.2.10 Score per residue for model 10

● Molecule 1: Type II secretion system core protein G





## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| 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                       | 1292           |
| Number of shifts mapped to atoms             | 1292           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 85%            |

## 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: CA

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.52±0.01    | 0±0/847 ( 0.0± 0.0%) | 0.88±0.01   | 0±1/1154 ( 0.0± 0.1%) |
| All | All   | 0.52         | 0/8470 ( 0.0%)       | 0.88        | 2/11540 ( 0.0%)       |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 92  | ASP  | CA-C-N | 5.50 | 124.96      | 119.24   | 7      | 1     |
| 1   | A     | 92  | ASP  | C-N-CA | 5.50 | 124.96      | 119.24   | 7      | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 824   | 791      | 789      | 35±4    |
| All | All   | 8250  | 7910     | 7890     | 353     |

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 22.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:43:LEU:HD22 | 1:A:64:LEU:HD11  | 0.87     | 1.47        | 9      | 8     |
| 1:A:50:TYR:HA   | 1:A:85:TYR:CE1   | 0.76     | 2.15        | 4      | 5     |
| 1:A:50:TYR:HA   | 1:A:85:TYR:CE2   | 0.74     | 2.17        | 6      | 3     |
| 1:A:67:LEU:HB3  | 1:A:86:ILE:HG23  | 0.69     | 1.64        | 6      | 8     |
| 1:A:33:ARG:O    | 1:A:37:ILE:HD13  | 0.69     | 1.88        | 8      | 10    |
| 1:A:54:ASN:OD1  | 1:A:77:PRO:HA    | 0.66     | 1.90        | 4      | 3     |
| 1:A:36:ALA:HB1  | 1:A:126:ILE:HG21 | 0.64     | 1.68        | 9      | 9     |
| 1:A:91:GLN:HA   | 1:A:98:TYR:OH    | 0.64     | 1.92        | 1      | 1     |
| 1:A:65:GLY:O    | 1:A:69:LYS:HB2   | 0.63     | 1.93        | 1      | 10    |
| 1:A:62:GLN:OE1  | 1:A:75:PRO:HD2   | 0.62     | 1.95        | 1      | 1     |
| 1:A:56:ARG:HD3  | 1:A:57:TYR:O     | 0.61     | 1.95        | 8      | 4     |
| 1:A:105:ARG:HD2 | 1:A:110:ASP:OD2  | 0.61     | 1.95        | 2      | 1     |
| 1:A:80:TYR:CG   | 1:A:81:PRO:HD2   | 0.61     | 2.31        | 8      | 1     |
| 1:A:66:ALA:HB1  | 1:A:71:PRO:HG3   | 0.59     | 1.75        | 10     | 6     |
| 1:A:92:ASP:CG   | 1:A:96:ALA:HB3   | 0.59     | 2.23        | 2      | 6     |
| 1:A:30:LYS:O    | 1:A:33:ARG:HG2   | 0.59     | 1.98        | 2      | 10    |
| 1:A:50:TYR:CD1  | 1:A:58:PRO:HG3   | 0.59     | 2.33        | 8      | 2     |
| 1:A:80:TYR:CD1  | 1:A:81:PRO:HD2   | 0.58     | 2.33        | 8      | 1     |
| 1:A:99:GLN:O    | 1:A:111:VAL:HA   | 0.58     | 1.98        | 8      | 7     |
| 1:A:32:ASP:O    | 1:A:93:PRO:HG2   | 0.57     | 1.99        | 10     | 1     |
| 1:A:80:TYR:HB3  | 1:A:85:TYR:CE2   | 0.57     | 2.35        | 2      | 6     |
| 1:A:127:GLY:O   | 1:A:131:VAL:HG22 | 0.56     | 2.00        | 8      | 8     |
| 1:A:71:PRO:HG2  | 1:A:77:PRO:CD    | 0.56     | 2.31        | 10     | 3     |
| 1:A:39:ASP:O    | 1:A:43:LEU:HG    | 0.55     | 2.01        | 1      | 10    |
| 1:A:127:GLY:C   | 1:A:131:VAL:HG22 | 0.55     | 2.26        | 3      | 10    |
| 1:A:44:GLU:CD   | 1:A:128:ASN:HB2  | 0.55     | 2.26        | 6      | 1     |
| 1:A:47:LEU:CD2  | 1:A:58:PRO:HG2   | 0.55     | 2.31        | 8      | 10    |
| 1:A:80:TYR:HB3  | 1:A:85:TYR:CE1   | 0.55     | 2.36        | 5      | 3     |
| 1:A:37:ILE:HG23 | 1:A:131:VAL:O    | 0.55     | 2.01        | 8      | 9     |
| 1:A:39:ASP:OD1  | 1:A:90:PRO:HB2   | 0.55     | 2.02        | 1      | 1     |
| 1:A:32:ASP:O    | 1:A:93:PRO:HG3   | 0.54     | 2.02        | 4      | 1     |
| 1:A:114:TYR:CD1 | 1:A:120:PRO:HB3  | 0.53     | 2.39        | 1      | 2     |
| 1:A:88:ARG:O    | 1:A:88:ARG:HD3   | 0.53     | 2.04        | 2      | 6     |
| 1:A:92:ASP:HB3  | 1:A:94:TRP:CE3   | 0.53     | 2.39        | 8      | 6     |
| 1:A:60:THR:HG23 | 1:A:100:LEU:O    | 0.52     | 2.03        | 8      | 10    |
| 1:A:94:TRP:CE2  | 1:A:116:PRO:HA   | 0.52     | 2.40        | 4      | 1     |
| 1:A:37:ILE:O    | 1:A:41:VAL:HG13  | 0.52     | 2.04        | 8      | 10    |
| 1:A:43:LEU:HB3  | 1:A:64:LEU:HD11  | 0.52     | 1.82        | 3      | 5     |
| 1:A:70:LYS:H    | 1:A:70:LYS:HD3   | 0.52     | 1.65        | 8      | 1     |
| 1:A:59:THR:OG1  | 1:A:62:GLN:HG3   | 0.51     | 2.05        | 1      | 9     |
| 1:A:100:LEU:CD1 | 1:A:109:VAL:HB   | 0.51     | 2.35        | 4      | 3     |
| 1:A:57:TYR:CD2  | 1:A:109:VAL:HG11 | 0.49     | 2.43        | 6      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:39:ASP:OD1   | 1:A:43:LEU:HD11  | 0.49     | 2.07        | 6      | 2     |
| 1:A:37:ILE:HG13  | 1:A:131:VAL:HB   | 0.49     | 1.84        | 4      | 10    |
| 1:A:50:TYR:CE1   | 1:A:58:PRO:HG3   | 0.49     | 2.42        | 8      | 1     |
| 1:A:30:LYS:O     | 1:A:34:GLN:HG2   | 0.49     | 2.06        | 8      | 2     |
| 1:A:119:MET:HA   | 1:A:119:MET:HE2  | 0.49     | 1.83        | 10     | 1     |
| 1:A:49:MET:HA    | 1:A:52:LEU:HD12  | 0.49     | 1.85        | 10     | 1     |
| 1:A:29:GLU:O     | 1:A:33:ARG:HB3   | 0.48     | 2.08        | 10     | 2     |
| 1:A:108:LYS:HG2  | 1:A:109:VAL:N    | 0.48     | 2.23        | 4      | 1     |
| 1:A:45:SER:O     | 1:A:49:MET:HG3   | 0.48     | 2.09        | 4      | 6     |
| 1:A:49:MET:HA    | 1:A:52:LEU:HB2   | 0.48     | 1.85        | 6      | 4     |
| 1:A:47:LEU:HB3   | 1:A:57:TYR:CE1   | 0.48     | 2.44        | 5      | 2     |
| 1:A:70:LYS:O     | 1:A:70:LYS:HD2   | 0.47     | 2.09        | 6      | 1     |
| 1:A:56:ARG:HD3   | 1:A:57:TYR:N     | 0.47     | 2.24        | 4      | 2     |
| 1:A:35:LYS:C     | 1:A:35:LYS:HD3   | 0.47     | 2.35        | 1      | 2     |
| 1:A:102:SER:HA   | 1:A:103:PRO:C    | 0.47     | 2.34        | 9      | 6     |
| 1:A:129:TRP:CD1  | 1:A:130:ASN:HD22 | 0.47     | 2.27        | 2      | 4     |
| 1:A:51:LYS:HB2   | 1:A:56:ARG:C     | 0.47     | 2.35        | 10     | 3     |
| 1:A:88:ARG:O     | 1:A:90:PRO:HD3   | 0.47     | 2.09        | 6      | 1     |
| 1:A:40:ILE:HA    | 1:A:43:LEU:CD1   | 0.47     | 2.40        | 7      | 7     |
| 1:A:66:ALA:CB    | 1:A:71:PRO:HG3   | 0.46     | 2.40        | 9      | 5     |
| 1:A:63:GLY:CA    | 1:A:100:LEU:HD23 | 0.46     | 2.41        | 5      | 3     |
| 1:A:46:ALA:CB    | 1:A:86:ILE:HG22  | 0.46     | 2.41        | 10     | 1     |
| 1:A:39:ASP:OD2   | 1:A:43:LEU:HD11  | 0.46     | 2.10        | 3      | 1     |
| 1:A:33:ARG:O     | 1:A:36:ALA:HB3   | 0.45     | 2.11        | 6      | 2     |
| 1:A:80:TYR:CB    | 1:A:85:TYR:CE1   | 0.45     | 2.99        | 5      | 3     |
| 1:A:63:GLY:O     | 1:A:67:LEU:HG    | 0.45     | 2.12        | 9      | 1     |
| 1:A:87:ARG:HA    | 1:A:87:ARG:NH1   | 0.45     | 2.26        | 2      | 1     |
| 1:A:100:LEU:HD11 | 1:A:109:VAL:HB   | 0.45     | 1.87        | 4      | 2     |
| 1:A:36:ALA:O     | 1:A:39:ASP:HB3   | 0.45     | 2.11        | 4      | 1     |
| 1:A:113:SER:O    | 1:A:126:ILE:HB   | 0.45     | 2.12        | 4      | 2     |
| 1:A:77:PRO:HB3   | 1:A:85:TYR:OH    | 0.45     | 2.12        | 9      | 1     |
| 1:A:67:LEU:O     | 1:A:84:GLY:HA3   | 0.44     | 2.12        | 9      | 1     |
| 1:A:36:ALA:HB2   | 1:A:92:ASP:OD2   | 0.44     | 2.12        | 9      | 1     |
| 1:A:117:ASP:HB3  | 1:A:124:ASP:OD2  | 0.44     | 2.11        | 8      | 1     |
| 1:A:60:THR:OG1   | 1:A:101:VAL:HA   | 0.44     | 2.13        | 10     | 3     |
| 1:A:129:TRP:NE1  | 1:A:130:ASN:HD22 | 0.44     | 2.10        | 9      | 6     |
| 1:A:117:ASP:OD2  | 1:A:119:MET:HB2  | 0.44     | 2.11        | 8      | 1     |
| 1:A:92:ASP:CB    | 1:A:96:ALA:HB3   | 0.44     | 2.42        | 10     | 2     |
| 1:A:92:ASP:HB3   | 1:A:94:TRP:CZ3   | 0.44     | 2.48        | 8      | 4     |
| 1:A:47:LEU:HD13  | 1:A:100:LEU:HD13 | 0.44     | 1.90        | 1      | 3     |
| 1:A:115:GLY:CA   | 1:A:126:ILE:HD13 | 0.44     | 2.42        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:131:VAL:HG23 | 1:A:132:GLY:N    | 0.44     | 2.27        | 10     | 1     |
| 1:A:47:LEU:HB3   | 1:A:57:TYR:CE2   | 0.43     | 2.48        | 10     | 1     |
| 1:A:70:LYS:H     | 1:A:70:LYS:CD    | 0.43     | 2.25        | 8      | 1     |
| 1:A:47:LEU:HD22  | 1:A:58:PRO:HG2   | 0.43     | 1.89        | 2      | 1     |
| 1:A:54:ASN:OD1   | 1:A:78:ARG:HD2   | 0.43     | 2.14        | 5      | 1     |
| 1:A:117:ASP:OD2  | 1:A:119:MET:HG2  | 0.43     | 2.13        | 9      | 1     |
| 1:A:40:ILE:HG21  | 1:A:128:ASN:HA   | 0.43     | 1.90        | 10     | 1     |
| 1:A:86:ILE:HD12  | 1:A:88:ARG:O     | 0.42     | 2.14        | 2      | 2     |
| 1:A:101:VAL:HG12 | 1:A:104:GLY:HA2  | 0.42     | 1.92        | 2      | 1     |
| 1:A:80:TYR:CB    | 1:A:85:TYR:CE2   | 0.42     | 3.02        | 2      | 1     |
| 1:A:37:ILE:CG1   | 1:A:131:VAL:HB   | 0.42     | 2.45        | 8      | 1     |
| 1:A:50:TYR:CD2   | 1:A:58:PRO:HG3   | 0.42     | 2.49        | 1      | 1     |
| 1:A:64:LEU:HG    | 1:A:98:TYR:CD1   | 0.42     | 2.50        | 9      | 1     |
| 1:A:47:LEU:HB3   | 1:A:57:TYR:CD1   | 0.42     | 2.50        | 5      | 1     |
| 1:A:119:MET:SD   | 1:A:122:THR:HG21 | 0.42     | 2.55        | 9      | 1     |
| 1:A:34:GLN:NE2   | 1:A:37:ILE:HG12  | 0.42     | 2.30        | 1      | 1     |
| 1:A:40:ILE:HG23  | 1:A:111:VAL:HG23 | 0.42     | 1.91        | 6      | 1     |
| 1:A:88:ARG:O     | 1:A:88:ARG:HD2   | 0.42     | 2.15        | 9      | 1     |
| 1:A:35:LYS:HD3   | 1:A:35:LYS:O     | 0.41     | 2.15        | 10     | 1     |
| 1:A:81:PRO:HB2   | 1:A:84:GLY:O     | 0.41     | 2.15        | 4      | 1     |
| 1:A:114:TYR:CD2  | 1:A:120:PRO:HB3  | 0.41     | 2.50        | 5      | 1     |
| 1:A:57:TYR:CD1   | 1:A:109:VAL:HG11 | 0.41     | 2.50        | 4      | 1     |
| 1:A:100:LEU:HD11 | 1:A:102:SER:HB2  | 0.41     | 1.90        | 4      | 1     |
| 1:A:66:ALA:CA    | 1:A:71:PRO:HG3   | 0.41     | 2.46        | 4      | 1     |
| 1:A:108:LYS:HD2  | 1:A:108:LYS:H    | 0.41     | 1.75        | 3      | 2     |
| 1:A:62:GLN:O     | 1:A:63:GLY:C     | 0.41     | 2.63        | 3      | 2     |
| 1:A:47:LEU:O     | 1:A:50:TYR:HB3   | 0.41     | 2.16        | 8      | 1     |
| 1:A:64:LEU:HD13  | 1:A:64:LEU:HA    | 0.40     | 1.78        | 6      | 1     |
| 1:A:122:THR:H    | 1:A:125:ASP:HB2  | 0.40     | 1.75        | 6      | 1     |
| 1:A:92:ASP:OD1   | 1:A:93:PRO:HD2   | 0.40     | 2.15        | 7      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|------------|-------------|----|
| 1   | A     | 105/125 (84%)   | 100±1 (95±1%) | 4±1 (4±1%) | 1±0 (1±0%) | 15          | 65 |
| All | All   | 1050/1250 (84%) | 995 (95%)     | 45 (4%)    | 10 (1%)    | 15          | 65 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 63  | GLY  | 10             |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed       | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|----------------|--------------|--------------|-------------|----|
| 1   | A     | 89/102 (87%)   | 74±1 (83±1%) | 15±1 (17±1%) | 4           | 39 |
| All | All   | 890/1020 (87%) | 741 (83%)    | 149 (17%)    | 4           | 39 |

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) |
|-----|-------|-----|------|----------------|
| 1   | A     | 37  | ILE  | 10             |
| 1   | A     | 41  | VAL  | 10             |
| 1   | A     | 43  | LEU  | 10             |
| 1   | A     | 51  | LYS  | 10             |
| 1   | A     | 100 | LEU  | 10             |
| 1   | A     | 109 | VAL  | 10             |
| 1   | A     | 52  | LEU  | 8              |
| 1   | A     | 53  | ASP  | 8              |
| 1   | A     | 94  | TRP  | 8              |
| 1   | A     | 99  | GLN  | 8              |
| 1   | A     | 88  | ARG  | 7              |
| 1   | A     | 98  | TYR  | 7              |
| 1   | A     | 108 | LYS  | 6              |
| 1   | A     | 78  | ARG  | 5              |
| 1   | A     | 64  | LEU  | 5              |
| 1   | A     | 105 | ARG  | 5              |
| 1   | A     | 35  | LYS  | 4              |
| 1   | A     | 56  | ARG  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 117 | ASP  | 2              |
| 1   | A     | 125 | ASP  | 2              |
| 1   | A     | 114 | TYR  | 2              |
| 1   | A     | 70  | LYS  | 2              |
| 1   | A     | 44  | GLU  | 1              |
| 1   | A     | 122 | THR  | 1              |
| 1   | A     | 48  | ASP  | 1              |
| 1   | A     | 92  | ASP  | 1              |
| 1   | A     | 89  | LEU  | 1              |
| 1   | A     | 80  | TYR  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 1 ligands modelled in this entry, 1 is 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 85% for the well-defined parts and 82% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_1*

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

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1292 |
| Number of shifts mapped to atoms        | 1292 |
| 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 117      | $-0.25 \pm 0.18$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 104      | $0.16 \pm 0.09$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 117      | $-0.06 \pm 0.16$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 106      | $0.49 \pm 0.19$                 | 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 85%, i.e. 1185 atoms were assigned a chemical shift out of a possible 1386. 5 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 507/513 (99%) | 205/209 (98%) | 208/210 (99%)   | 94/94 (100%)    |
| Sidechain | 618/777 (80%) | 412/499 (83%) | 199/245 (81%)   | 7/33 (21%)      |

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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 | 60/96 (62%)     | 30/45 (67%)          | 28/47 (60%)           | 2/4 (50%)             |
| Overall  | 1185/1386 (85%) | 647/753 (86%)        | 435/502 (87%)         | 103/131 (79%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1292 atoms were assigned a chemical shift out of a possible 1584. 5 out of 13 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  | 569/617 (92%)   | 229/254 (90%)        | 234/250 (94%)         | 106/113 (94%)         |
| Sidechain | 659/863 (76%)   | 439/554 (79%)        | 211/271 (78%)         | 9/38 (24%)            |
| Aromatic  | 64/104 (62%)    | 32/49 (65%)          | 30/49 (61%)           | 2/6 (33%)             |
| Overall   | 1292/1584 (82%) | 700/857 (82%)        | 475/570 (83%)         | 117/157 (75%)         |

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

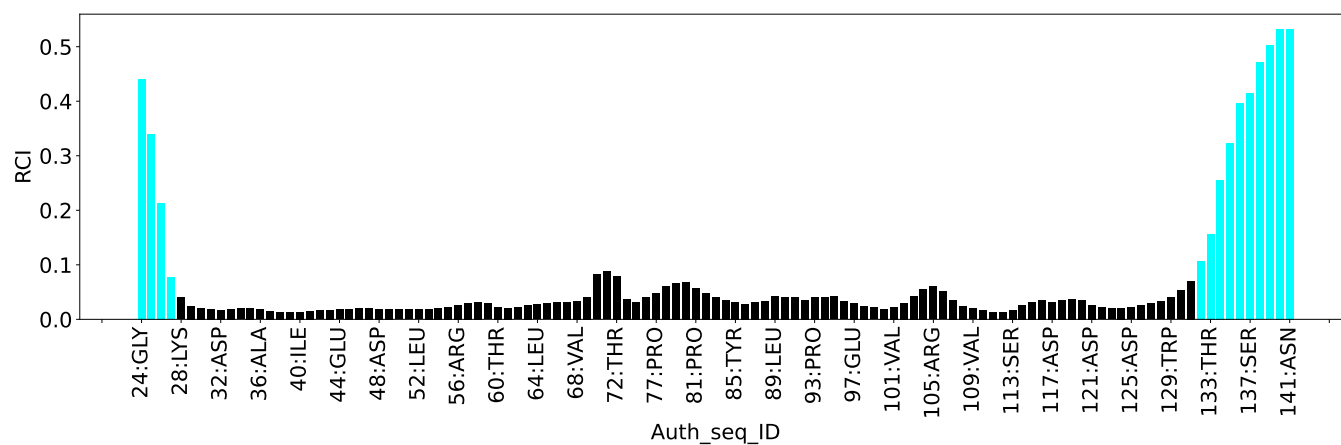
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 127 | GLY  | HA3  | 1.52       | 2.08 – 5.71         | -6.5    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1601  |
| Intra-residue ( $ i-j =0$ )                              | 584   |
| Sequential ( $ i-j =1$ )                                 | 383   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 300   |
| Long range ( $ i-j \geq 5$ )                             | 331   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 173   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 14.1  |
| Number of long range restraints per residue <sup>1</sup> | 2.6   |

<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)  | 79.7                                   | 0.2     |
| 0.2-0.5 (Medium) | 145.2                                  | 0.5     |
| >0.5 (Large)     | 109.6                                  | 2.92    |

### 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)   | 14.7                                   | 6.23    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

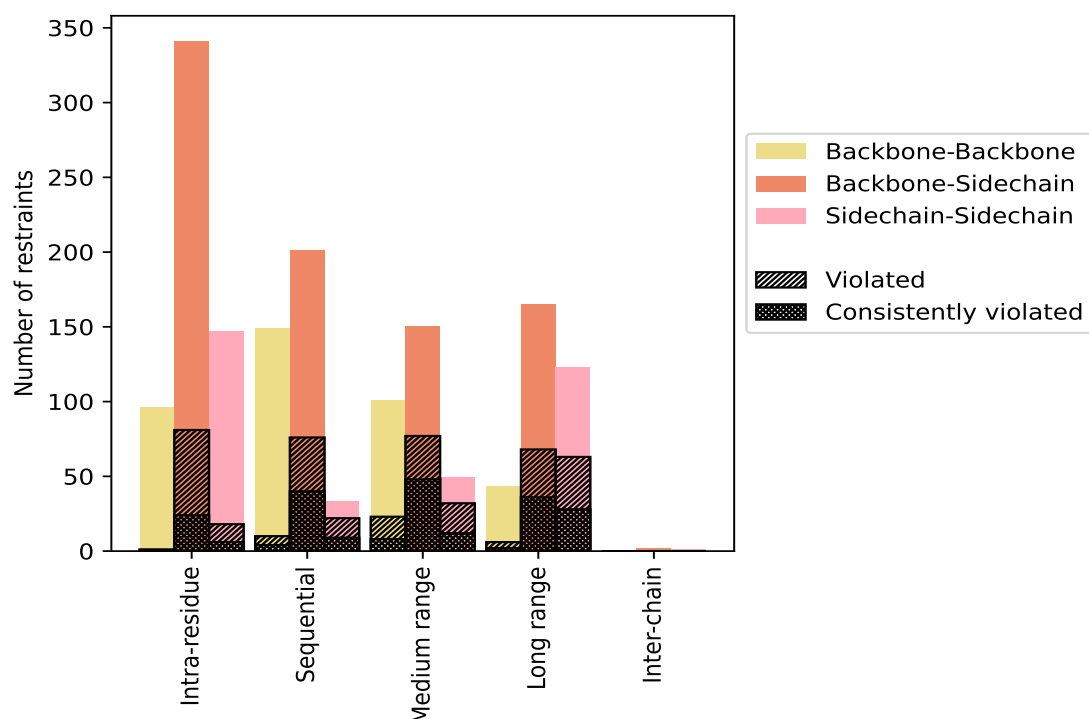
### 9.1 Summary of distance violations ⓘ

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>584</b>  | <b>36.5</b>    | <b>100</b>            | <b>17.1</b>    | <b>6.2</b>     | <b>31</b>                          | <b>5.3</b>     | <b>1.9</b>     |
| Backbone-Backbone                                                           | 96          | 6.0            | 1                     | 1.0            | 0.1            | 1                                  | 1.0            | 0.1            |
| Backbone-Sidechain                                                          | 341         | 21.3           | 81                    | 23.8           | 5.1            | 24                                 | 7.0            | 1.5            |
| Sidechain-Sidechain                                                         | 147         | 9.2            | 18                    | 12.2           | 1.1            | 6                                  | 4.1            | 0.4            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>383</b>  | <b>23.9</b>    | <b>108</b>            | <b>28.2</b>    | <b>6.7</b>     | <b>53</b>                          | <b>13.8</b>    | <b>3.3</b>     |
| Backbone-Backbone                                                           | 149         | 9.3            | 10                    | 6.7            | 0.6            | 4                                  | 2.7            | 0.2            |
| Backbone-Sidechain                                                          | 201         | 12.6           | 76                    | 37.8           | 4.7            | 40                                 | 19.9           | 2.5            |
| Sidechain-Sidechain                                                         | 33          | 2.1            | 22                    | 66.7           | 1.4            | 9                                  | 27.3           | 0.6            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>300</b>  | <b>18.7</b>    | <b>132</b>            | <b>44.0</b>    | <b>8.2</b>     | <b>68</b>                          | <b>22.7</b>    | <b>4.2</b>     |
| Backbone-Backbone                                                           | 101         | 6.3            | 23                    | 22.8           | 1.4            | 8                                  | 7.9            | 0.5            |
| Backbone-Sidechain                                                          | 150         | 9.4            | 77                    | 51.3           | 4.8            | 48                                 | 32.0           | 3.0            |
| Sidechain-Sidechain                                                         | 49          | 3.1            | 32                    | 65.3           | 2.0            | 12                                 | 24.5           | 0.7            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>331</b>  | <b>20.7</b>    | <b>137</b>            | <b>41.4</b>    | <b>8.6</b>     | <b>66</b>                          | <b>19.9</b>    | <b>4.1</b>     |
| Backbone-Backbone                                                           | 43          | 2.7            | 6                     | 14.0           | 0.4            | 2                                  | 4.7            | 0.1            |
| Backbone-Sidechain                                                          | 165         | 10.3           | 68                    | 41.2           | 4.2            | 36                                 | 21.8           | 2.2            |
| Sidechain-Sidechain                                                         | 123         | 7.7            | 63                    | 51.2           | 3.9            | 28                                 | 22.8           | 1.7            |
| <b>Inter-chain</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>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1601</b> | <b>100.0</b>   | <b>477</b>            | <b>29.8</b>    | <b>29.8</b>    | <b>218</b>                         | <b>13.6</b>    | <b>13.6</b>    |
| Backbone-Backbone                                                           | 389         | 24.3           | 40                    | 10.3           | 2.5            | 15                                 | 3.9            | 0.9            |
| Backbone-Sidechain                                                          | 859         | 53.7           | 302                   | 35.2           | 18.9           | 148                                | 17.2           | 9.2            |
| Sidechain-Sidechain                                                         | 353         | 22.0           | 135                   | 38.2           | 8.4            | 55                                 | 15.6           | 3.4            |

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

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



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

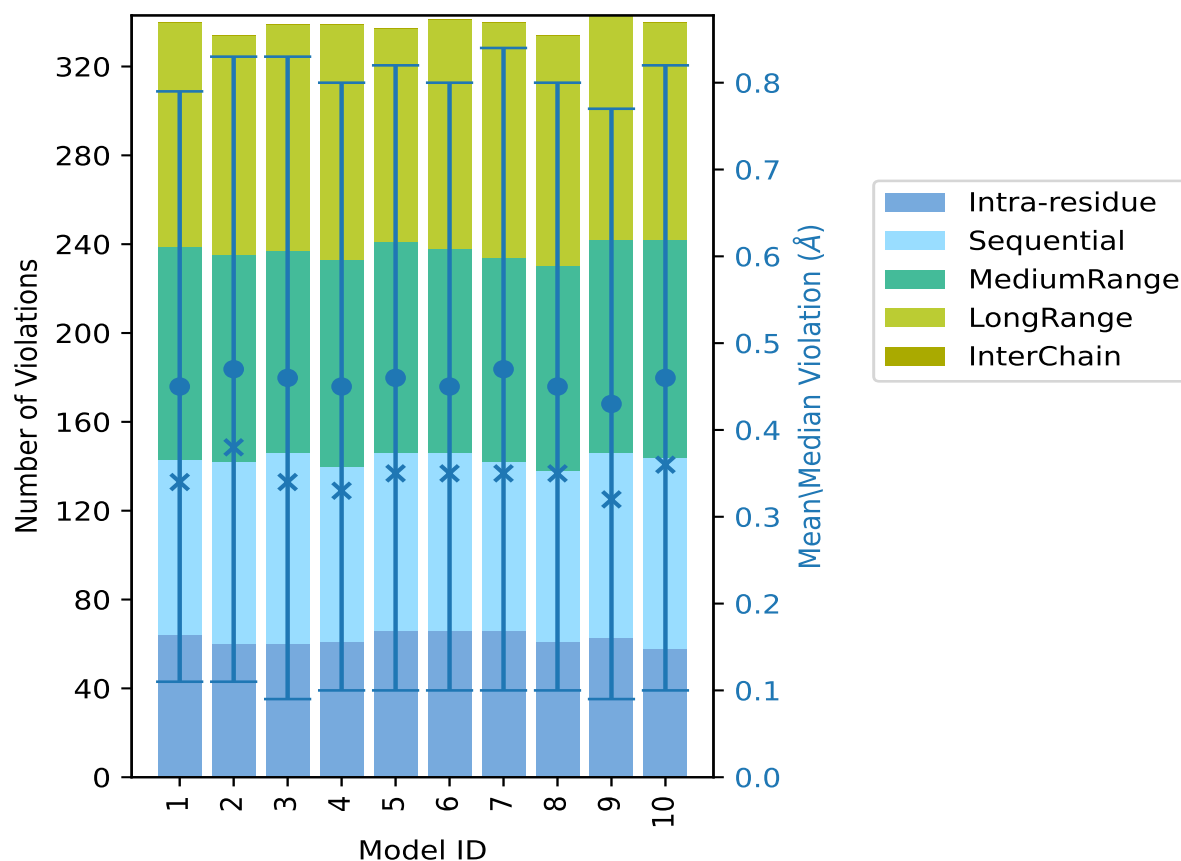
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 64                   | 79              | 96              | 101             | 0               | 340   | 0.45     | 2.63    | 0.34                | 0.34       |
| 2        | 60                   | 82              | 93              | 99              | 0               | 334   | 0.47     | 2.85    | 0.36                | 0.38       |
| 3        | 60                   | 86              | 91              | 102             | 0               | 339   | 0.46     | 2.92    | 0.37                | 0.34       |
| 4        | 61                   | 79              | 93              | 106             | 0               | 339   | 0.45     | 2.89    | 0.35                | 0.33       |
| 5        | 66                   | 80              | 95              | 96              | 0               | 337   | 0.46     | 2.9     | 0.36                | 0.35       |
| 6        | 66                   | 80              | 92              | 103             | 0               | 341   | 0.45     | 2.85    | 0.35                | 0.35       |
| 7        | 66                   | 76              | 92              | 106             | 0               | 340   | 0.47     | 2.83    | 0.37                | 0.35       |
| 8        | 61                   | 77              | 92              | 104             | 0               | 334   | 0.45     | 2.86    | 0.35                | 0.35       |
| 9        | 63                   | 83              | 96              | 101             | 0               | 343   | 0.43     | 2.89    | 0.34                | 0.32       |
| 10       | 58                   | 86              | 98              | 98              | 0               | 340   | 0.46     | 2.82    | 0.36                | 0.36       |

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1121(IR:484, SQ:275, MR:168, LR:194, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 17                            | 14              | 13              | 14              | 0               | 58    | 1                        | 10.0 |
| 10                            | 2               | 8               | 9               | 0               | 29    | 2                        | 20.0 |
| 7                             | 10              | 5               | 7               | 0               | 29    | 3                        | 30.0 |

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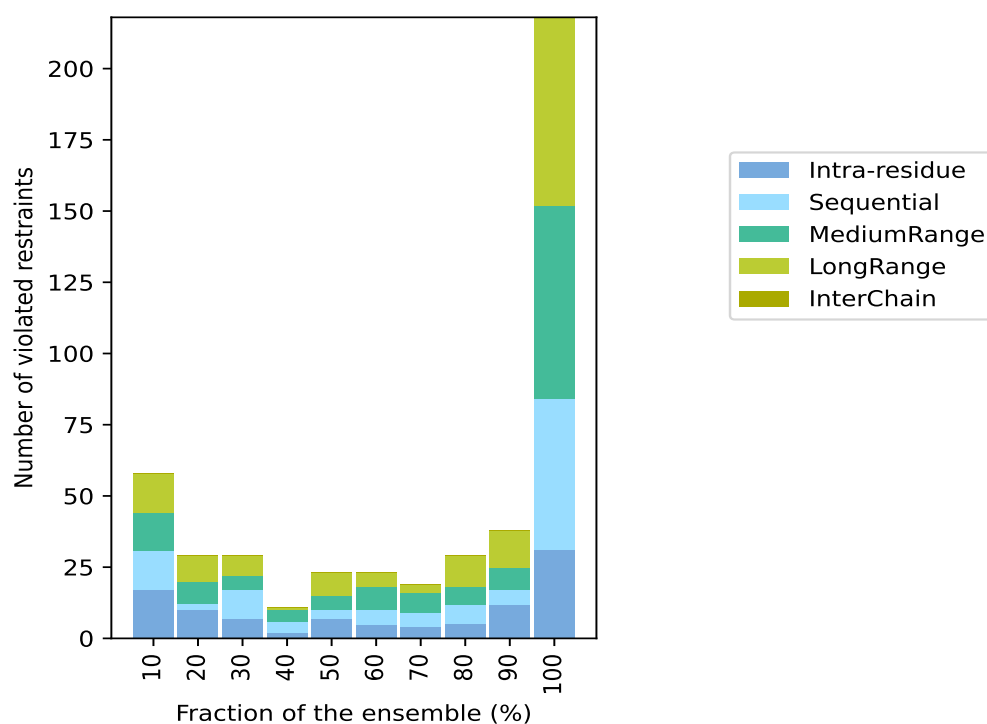
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 2                             | 4               | 4               | 1               | 0               | 11    | 4                        | 40.0  |
| 7                             | 3               | 5               | 8               | 0               | 23    | 5                        | 50.0  |
| 5                             | 5               | 8               | 5               | 0               | 23    | 6                        | 60.0  |
| 4                             | 5               | 7               | 3               | 0               | 19    | 7                        | 70.0  |
| 5                             | 7               | 6               | 11              | 0               | 29    | 8                        | 80.0  |
| 12                            | 5               | 8               | 13              | 0               | 38    | 9                        | 90.0  |
| 31                            | 53              | 68              | 66              | 0               | 218   | 10                       | 100.0 |

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

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

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



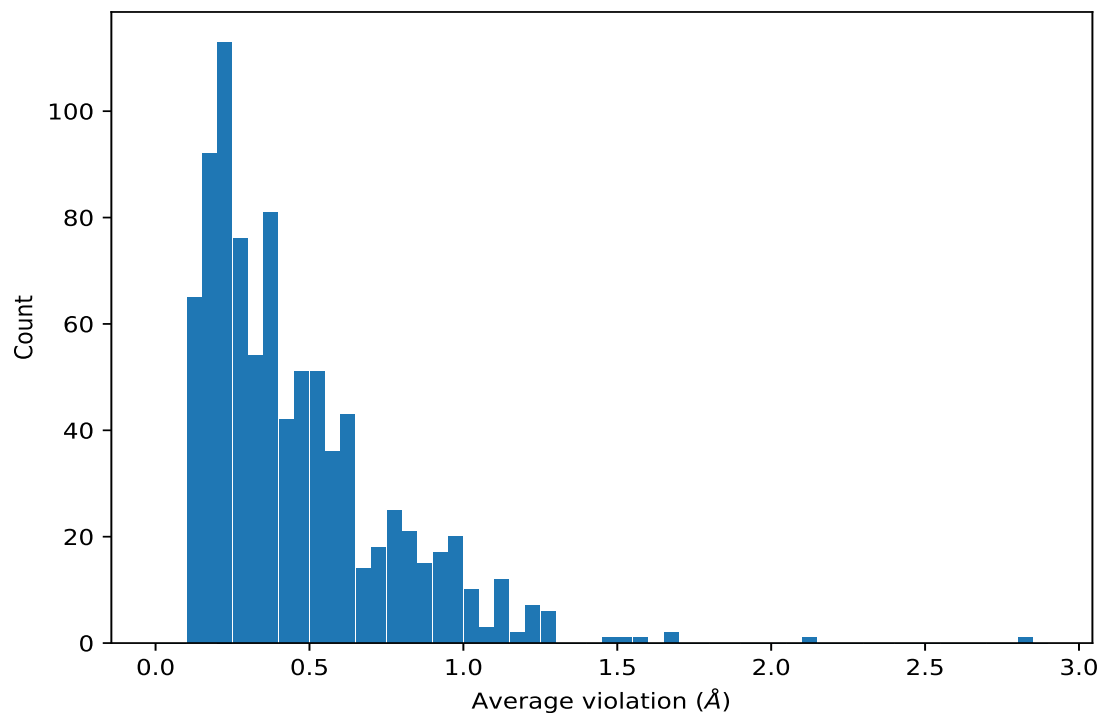
## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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



in the ensemble



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

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

| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1357) | 1:62:A:GLN:HE21  | 1:63:A:GLY:HA3  | 10                  | 2.84     | 0.08                | 2.86       |
| (1,341)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB2  | 10                  | 2.11     | 0.1                 | 2.12       |
| (1,541)  | 1:85:A:TYR:HE1   | 1:84:A:GLY:HA3  | 10                  | 1.65     | 0.13                | 1.69       |
| (1,541)  | 1:85:A:TYR:HE2   | 1:84:A:GLY:HA3  | 10                  | 1.65     | 0.13                | 1.69       |
| (1,768)  | 1:67:A:LEU:HB2   | 1:85:A:TYR:HB3  | 10                  | 1.58     | 0.15                | 1.6        |
| (1,51)   | 1:33:A:ARG:HB3   | 1:116:A:PRO:HG2 | 10                  | 1.51     | 0.14                | 1.52       |
| (1,1186) | 1:62:A:GLN:HE22  | 1:75:A:PRO:HB2  | 10                  | 1.47     | 0.25                | 1.5        |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA  | 10                  | 1.29     | 0.06                | 1.3        |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG   | 10                  | 1.27     | 0.07                | 1.29       |
| (1,1520) | 1:111:A:VAL:HG11 | 1:110:A:ASP:HB2 | 10                  | 1.26     | 0.07                | 1.22       |
| (1,1520) | 1:111:A:VAL:HG12 | 1:110:A:ASP:HB2 | 10                  | 1.26     | 0.07                | 1.22       |
| (1,1520) | 1:111:A:VAL:HG13 | 1:110:A:ASP:HB2 | 10                  | 1.26     | 0.07                | 1.22       |
| (1,1520) | 1:111:A:VAL:HG12 | 1:128:A:ASN:HB2 | 10                  | 1.26     | 0.07                | 1.22       |
| (1,1505) | 1:66:A:ALA:HB3   | 1:63:A:GLY:HA3  | 10                  | 1.23     | 0.03                | 1.23       |
| (1,1505) | 1:66:A:ALA:HB2   | 1:64:A:LEU:HA   | 10                  | 1.23     | 0.03                | 1.23       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1505) | 1:66:A:ALA:HB1  | 1:63:A:GLY:HA3   | 10                  | 1.23     | 0.03                | 1.23       |
| (1,1505) | 1:66:A:ALA:HB2  | 1:63:A:GLY:HA3   | 10                  | 1.23     | 0.03                | 1.23       |
| (1,1505) | 1:66:A:ALA:HB1  | 1:64:A:LEU:HA    | 10                  | 1.23     | 0.03                | 1.23       |
| (1,1417) | 1:33:A:ARG:H    | 1:116:A:PRO:HG2  | 10                  | 1.22     | 0.18                | 1.19       |
| (1,794)  | 1:106:A:HIS:HB3 | 1:105:A:ARG:H    | 10                  | 1.19     | 0.07                | 1.17       |
| (1,1180) | 1:118:A:GLY:H   | 1:119:A:MET:HB3  | 10                  | 1.18     | 0.32                | 1.26       |
| (1,787)  | 1:96:A:ALA:HB1  | 1:114:A:TYR:HB3  | 10                  | 1.13     | 0.41                | 1.1        |
| (1,787)  | 1:96:A:ALA:HB3  | 1:114:A:TYR:HB3  | 10                  | 1.13     | 0.41                | 1.1        |
| (1,787)  | 1:96:A:ALA:HB2  | 1:114:A:TYR:HB3  | 10                  | 1.13     | 0.41                | 1.1        |
| (1,432)  | 1:41:A:VAL:HG11 | 1:42:A:ALA:HB2   | 10                  | 1.13     | 0.04                | 1.13       |
| (1,432)  | 1:41:A:VAL:HG13 | 1:42:A:ALA:HB3   | 10                  | 1.13     | 0.04                | 1.13       |
| (1,432)  | 1:41:A:VAL:HG11 | 1:42:A:ALA:HB1   | 10                  | 1.13     | 0.04                | 1.13       |
| (1,432)  | 1:41:A:VAL:HG13 | 1:42:A:ALA:HB1   | 10                  | 1.13     | 0.04                | 1.13       |
| (1,432)  | 1:41:A:VAL:HG11 | 1:42:A:ALA:HB3   | 10                  | 1.13     | 0.04                | 1.13       |
| (1,432)  | 1:41:A:VAL:HG12 | 1:42:A:ALA:HB1   | 10                  | 1.13     | 0.04                | 1.13       |
| (1,1307) | 1:110:A:ASP:H   | 1:100:A:LEU:HB3  | 10                  | 1.05     | 0.03                | 1.06       |
| (1,801)  | 1:79:A:SER:HB3  | 1:78:A:ARG:HB2   | 10                  | 1.04     | 0.47                | 1.07       |
| (1,229)  | 1:63:A:GLY:HA2  | 1:111:A:VAL:HG12 | 10                  | 1.03     | 0.09                | 1.01       |
| (1,229)  | 1:63:A:GLY:HA2  | 1:111:A:VAL:HG13 | 10                  | 1.03     | 0.09                | 1.01       |
| (1,229)  | 1:63:A:GLY:HA2  | 1:111:A:VAL:HG11 | 10                  | 1.03     | 0.09                | 1.01       |
| (1,1430) | 1:47:A:LEU:H    | 1:64:A:LEU:HD11  | 10                  | 1.02     | 0.15                | 0.97       |
| (1,1430) | 1:47:A:LEU:H    | 1:64:A:LEU:HD13  | 10                  | 1.02     | 0.15                | 0.97       |
| (1,1430) | 1:47:A:LEU:H    | 1:64:A:LEU:HD22  | 10                  | 1.02     | 0.15                | 0.97       |
| (1,1430) | 1:47:A:LEU:H    | 1:64:A:LEU:HD12  | 10                  | 1.02     | 0.15                | 0.97       |
| (1,1250) | 1:94:A:TRP:HE1  | 1:116:A:PRO:HG2  | 10                  | 1.0      | 0.13                | 1.04       |
| (1,1535) | 1:62:A:GLN:H    | 1:66:A:ALA:HB1   | 10                  | 0.99     | 0.08                | 1.03       |
| (1,1535) | 1:62:A:GLN:H    | 1:66:A:ALA:HB3   | 10                  | 0.99     | 0.08                | 1.03       |
| (1,1535) | 1:62:A:GLN:H    | 1:60:A:THR:HG23  | 10                  | 0.99     | 0.08                | 1.03       |
| (1,1535) | 1:62:A:GLN:H    | 1:66:A:ALA:HB2   | 10                  | 0.99     | 0.08                | 1.03       |
| (1,1212) | 1:62:A:GLN:H    | 1:62:A:GLN:HE21  | 10                  | 0.99     | 0.02                | 0.98       |
| (1,1554) | 1:66:A:ALA:H    | 1:64:A:LEU:HB2   | 10                  | 0.97     | 0.02                | 0.97       |
| (1,1554) | 1:66:A:ALA:H    | 1:58:A:PRO:HB3   | 10                  | 0.97     | 0.02                | 0.97       |
| (1,1554) | 1:66:A:ALA:H    | 1:64:A:LEU:HB3   | 10                  | 0.97     | 0.02                | 0.97       |
| (1,1527) | 1:66:A:ALA:HB3  | 1:68:A:VAL:H     | 10                  | 0.95     | 0.03                | 0.96       |
| (1,1527) | 1:66:A:ALA:HB2  | 1:68:A:VAL:H     | 10                  | 0.95     | 0.03                | 0.96       |
| (1,1527) | 1:66:A:ALA:HB1  | 1:68:A:VAL:H     | 10                  | 0.95     | 0.03                | 0.96       |
| (1,898)  | 1:52:A:LEU:HD23 | 1:53:A:ASP:H     | 10                  | 0.95     | 0.07                | 0.94       |
| (1,898)  | 1:52:A:LEU:HD22 | 1:53:A:ASP:H     | 10                  | 0.95     | 0.07                | 0.94       |
| (1,898)  | 1:52:A:LEU:HD11 | 1:53:A:ASP:H     | 10                  | 0.95     | 0.07                | 0.94       |
| (1,898)  | 1:52:A:LEU:HD12 | 1:53:A:ASP:H     | 10                  | 0.95     | 0.07                | 0.94       |
| (1,898)  | 1:52:A:LEU:HD21 | 1:53:A:ASP:H     | 10                  | 0.95     | 0.07                | 0.94       |
| (1,898)  | 1:52:A:LEU:HD13 | 1:53:A:ASP:H     | 10                  | 0.95     | 0.07                | 0.94       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG22 | 10                  | 0.94     | 0.08                | 0.96       |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG21 | 10                  | 0.94     | 0.08                | 0.96       |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG23 | 10                  | 0.94     | 0.08                | 0.96       |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 10                  | 0.93     | 0.05                | 0.92       |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG13 | 10                  | 0.92     | 0.06                | 0.93       |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG12 | 10                  | 0.92     | 0.06                | 0.93       |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG11 | 10                  | 0.92     | 0.06                | 0.93       |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD12  | 10                  | 0.9      | 0.22                | 0.82       |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD11  | 10                  | 0.9      | 0.22                | 0.82       |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD23  | 10                  | 0.9      | 0.22                | 0.82       |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD13  | 10                  | 0.9      | 0.22                | 0.82       |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG23  | 10                  | 0.9      | 0.06                | 0.9        |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG22  | 10                  | 0.9      | 0.06                | 0.9        |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG21  | 10                  | 0.9      | 0.06                | 0.9        |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG3   | 10                  | 0.89     | 0.12                | 0.9        |
| (1,99)   | 1:38:A:SER:HB2   | 1:90:A:PRO:HG2   | 10                  | 0.89     | 0.12                | 0.9        |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG2   | 10                  | 0.89     | 0.12                | 0.9        |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 10                  | 0.89     | 0.03                | 0.9        |
| (1,809)  | 1:100:A:LEU:HD13 | 1:63:A:GLY:H     | 10                  | 0.89     | 0.03                | 0.9        |
| (1,809)  | 1:100:A:LEU:HD12 | 1:63:A:GLY:H     | 10                  | 0.89     | 0.03                | 0.9        |
| (1,301)  | 1:73:A:THR:HG21  | 1:76:A:GLU:HB3   | 10                  | 0.86     | 0.05                | 0.86       |
| (1,301)  | 1:73:A:THR:HG22  | 1:76:A:GLU:HB3   | 10                  | 0.86     | 0.05                | 0.86       |
| (1,301)  | 1:73:A:THR:HG23  | 1:76:A:GLU:HB3   | 10                  | 0.86     | 0.05                | 0.86       |
| (1,647)  | 1:42:A:ALA:HB1   | 1:43:A:LEU:HD12  | 10                  | 0.85     | 0.02                | 0.84       |
| (1,647)  | 1:42:A:ALA:HB2   | 1:43:A:LEU:HD11  | 10                  | 0.85     | 0.02                | 0.84       |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD13  | 10                  | 0.85     | 0.02                | 0.84       |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD11  | 10                  | 0.85     | 0.02                | 0.84       |
| (1,647)  | 1:42:A:ALA:HB2   | 1:43:A:LEU:HD13  | 10                  | 0.85     | 0.02                | 0.84       |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD12  | 10                  | 0.85     | 0.02                | 0.84       |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG23  | 10                  | 0.84     | 0.04                | 0.84       |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG22  | 10                  | 0.84     | 0.04                | 0.84       |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG21  | 10                  | 0.84     | 0.04                | 0.84       |
| (1,736)  | 1:86:A:ILE:HG23  | 1:85:A:TYR:HD1   | 10                  | 0.82     | 0.17                | 0.87       |
| (1,736)  | 1:86:A:ILE:HG21  | 1:85:A:TYR:HD2   | 10                  | 0.82     | 0.17                | 0.87       |
| (1,736)  | 1:86:A:ILE:HG23  | 1:85:A:TYR:HD2   | 10                  | 0.82     | 0.17                | 0.87       |
| (1,736)  | 1:86:A:ILE:HG21  | 1:85:A:TYR:HD1   | 10                  | 0.82     | 0.17                | 0.87       |
| (1,736)  | 1:86:A:ILE:HG22  | 1:85:A:TYR:HD1   | 10                  | 0.82     | 0.17                | 0.87       |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB3   | 10                  | 0.81     | 0.05                | 0.82       |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB1   | 10                  | 0.81     | 0.05                | 0.82       |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB2   | 10                  | 0.81     | 0.05                | 0.82       |
| (1,665)  | 1:109:A:VAL:HG22 | 1:102:A:SER:HB2  | 10                  | 0.81     | 0.07                | 0.79       |
| (1,665)  | 1:109:A:VAL:HG21 | 1:102:A:SER:HB2  | 10                  | 0.81     | 0.07                | 0.79       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,665)  | 1:109:A:VAL:HG23 | 1:102:A:SER:HB2  | 10                  | 0.81     | 0.07                | 0.79       |
| (1,1524) | 1:60:A:THR:HB    | 1:101:A:VAL:HG23 | 10                  | 0.81     | 0.04                | 0.82       |
| (1,1524) | 1:60:A:THR:HB    | 1:100:A:LEU:HG   | 10                  | 0.81     | 0.04                | 0.82       |
| (1,1524) | 1:60:A:THR:HB    | 1:101:A:VAL:HG21 | 10                  | 0.81     | 0.04                | 0.82       |
| (1,1524) | 1:60:A:THR:HB    | 1:101:A:VAL:HG22 | 10                  | 0.81     | 0.04                | 0.82       |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG23 | 10                  | 0.79     | 0.07                | 0.8        |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG22 | 10                  | 0.79     | 0.07                | 0.8        |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG21 | 10                  | 0.79     | 0.07                | 0.8        |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 10                  | 0.78     | 0.04                | 0.8        |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 10                  | 0.78     | 0.06                | 0.77       |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG12  | 10                  | 0.78     | 0.03                | 0.78       |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG11  | 10                  | 0.78     | 0.03                | 0.78       |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG13  | 10                  | 0.78     | 0.03                | 0.78       |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 10                  | 0.77     | 0.12                | 0.74       |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 10                  | 0.77     | 0.35                | 0.66       |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB3   | 10                  | 0.77     | 0.35                | 0.66       |
| (1,619)  | 1:100:A:LEU:HD23 | 1:100:A:LEU:HA   | 10                  | 0.77     | 0.02                | 0.76       |
| (1,619)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:HA   | 10                  | 0.77     | 0.02                | 0.76       |
| (1,619)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:HA   | 10                  | 0.77     | 0.02                | 0.76       |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB1   | 10                  | 0.76     | 0.04                | 0.76       |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB2   | 10                  | 0.76     | 0.04                | 0.76       |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB3   | 10                  | 0.76     | 0.04                | 0.76       |
| (1,361)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HA   | 10                  | 0.76     | 0.11                | 0.75       |
| (1,361)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HA   | 10                  | 0.76     | 0.11                | 0.75       |
| (1,281)  | 1:40:A:ILE:HD11  | 1:41:A:VAL:H     | 10                  | 0.75     | 0.02                | 0.75       |
| (1,281)  | 1:40:A:ILE:HD13  | 1:41:A:VAL:H     | 10                  | 0.75     | 0.02                | 0.75       |
| (1,281)  | 1:40:A:ILE:HD12  | 1:41:A:VAL:H     | 10                  | 0.75     | 0.02                | 0.75       |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB2   | 10                  | 0.73     | 0.07                | 0.74       |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB3   | 10                  | 0.73     | 0.07                | 0.74       |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB1   | 10                  | 0.73     | 0.07                | 0.74       |
| (1,661)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HG12  | 10                  | 0.71     | 0.08                | 0.7        |
| (1,661)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HG12  | 10                  | 0.71     | 0.08                | 0.7        |
| (1,661)  | 1:111:A:VAL:HG21 | 1:40:A:ILE:HG12  | 10                  | 0.71     | 0.08                | 0.7        |
| (1,1541) | 1:86:A:ILE:HG21  | 1:87:A:ARG:H     | 10                  | 0.71     | 0.08                | 0.7        |
| (1,1541) | 1:86:A:ILE:HG22  | 1:87:A:ARG:H     | 10                  | 0.71     | 0.08                | 0.7        |
| (1,1541) | 1:86:A:ILE:HG23  | 1:87:A:ARG:H     | 10                  | 0.71     | 0.08                | 0.7        |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG22  | 10                  | 0.7      | 0.12                | 0.73       |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG21  | 10                  | 0.7      | 0.12                | 0.73       |
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG22  | 10                  | 0.7      | 0.12                | 0.73       |
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG23  | 10                  | 0.7      | 0.12                | 0.73       |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG23  | 10                  | 0.7      | 0.12                | 0.73       |
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG21  | 10                  | 0.7      | 0.12                | 0.73       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,737)  | 1:40:A:ILE:HD12  | 1:128:A:ASN:H    | 10                  | 0.69     | 0.03                | 0.68       |
| (1,737)  | 1:40:A:ILE:HD13  | 1:128:A:ASN:H    | 10                  | 0.69     | 0.03                | 0.68       |
| (1,737)  | 1:40:A:ILE:HD11  | 1:128:A:ASN:H    | 10                  | 0.69     | 0.03                | 0.68       |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 10                  | 0.69     | 0.2                 | 0.72       |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 10                  | 0.66     | 0.03                | 0.66       |
| (1,1493) | 1:109:A:VAL:HG12 | 1:108:A:LYS:H    | 10                  | 0.66     | 0.12                | 0.62       |
| (1,1493) | 1:109:A:VAL:HG11 | 1:108:A:LYS:H    | 10                  | 0.66     | 0.12                | 0.62       |
| (1,1493) | 1:109:A:VAL:HG13 | 1:108:A:LYS:H    | 10                  | 0.66     | 0.12                | 0.62       |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG21  | 10                  | 0.65     | 0.02                | 0.65       |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG22  | 10                  | 0.65     | 0.02                | 0.65       |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG23  | 10                  | 0.65     | 0.02                | 0.65       |
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 10                  | 0.65     | 0.12                | 0.68       |
| (1,1543) | 1:64:A:LEU:HD12  | 1:67:A:LEU:H     | 10                  | 0.65     | 0.12                | 0.68       |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 10                  | 0.62     | 0.03                | 0.62       |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD13 | 10                  | 0.62     | 0.03                | 0.62       |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD12 | 10                  | 0.62     | 0.03                | 0.62       |
| (1,641)  | 1:46:A:ALA:HB3   | 1:45:A:SER:H     | 10                  | 0.62     | 0.04                | 0.62       |
| (1,641)  | 1:46:A:ALA:HB1   | 1:45:A:SER:H     | 10                  | 0.62     | 0.04                | 0.62       |
| (1,641)  | 1:46:A:ALA:HB2   | 1:45:A:SER:H     | 10                  | 0.62     | 0.04                | 0.62       |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG13 | 10                  | 0.62     | 0.15                | 0.62       |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG12 | 10                  | 0.62     | 0.15                | 0.62       |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG11 | 10                  | 0.62     | 0.15                | 0.62       |
| (1,194)  | 1:111:A:VAL:HG13 | 1:43:A:LEU:HD11  | 10                  | 0.62     | 0.04                | 0.62       |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD13  | 10                  | 0.62     | 0.04                | 0.62       |
| (1,194)  | 1:111:A:VAL:HG12 | 1:43:A:LEU:HD12  | 10                  | 0.62     | 0.04                | 0.62       |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD12  | 10                  | 0.62     | 0.04                | 0.62       |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD11  | 10                  | 0.62     | 0.04                | 0.62       |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 10                  | 0.61     | 0.37                | 0.5        |
| (1,642)  | 1:46:A:ALA:HB2   | 1:85:A:TYR:HD2   | 10                  | 0.61     | 0.14                | 0.59       |
| (1,642)  | 1:46:A:ALA:HB2   | 1:85:A:TYR:HD1   | 10                  | 0.61     | 0.14                | 0.59       |
| (1,642)  | 1:46:A:ALA:HB3   | 1:85:A:TYR:HD1   | 10                  | 0.61     | 0.14                | 0.59       |
| (1,642)  | 1:46:A:ALA:HB3   | 1:85:A:TYR:HD2   | 10                  | 0.61     | 0.14                | 0.59       |
| (1,642)  | 1:46:A:ALA:HB1   | 1:85:A:TYR:HD2   | 10                  | 0.61     | 0.14                | 0.59       |
| (1,642)  | 1:46:A:ALA:HB1   | 1:85:A:TYR:HD1   | 10                  | 0.61     | 0.14                | 0.59       |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 10                  | 0.61     | 0.02                | 0.61       |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD21  | 10                  | 0.61     | 0.07                | 0.6        |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD22  | 10                  | 0.61     | 0.07                | 0.6        |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD23  | 10                  | 0.61     | 0.07                | 0.6        |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB3   | 10                  | 0.61     | 0.03                | 0.62       |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB2   | 10                  | 0.61     | 0.03                | 0.62       |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB1   | 10                  | 0.61     | 0.03                | 0.62       |
| (1,765)  | 1:37:A:ILE:HD12  | 1:33:A:ARG:H     | 10                  | 0.6      | 0.04                | 0.61       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,765)  | 1:37:A:ILE:HD11 | 1:33:A:ARG:H     | 10                  | 0.6      | 0.04                | 0.61       |
| (1,765)  | 1:37:A:ILE:HD13 | 1:33:A:ARG:H     | 10                  | 0.6      | 0.04                | 0.61       |
| (1,359)  | 1:64:A:LEU:HD11 | 1:67:A:LEU:H     | 10                  | 0.6      | 0.12                | 0.64       |
| (1,359)  | 1:64:A:LEU:HD12 | 1:67:A:LEU:H     | 10                  | 0.6      | 0.12                | 0.64       |
| (1,890)  | 1:41:A:VAL:H    | 1:42:A:ALA:HB2   | 10                  | 0.6      | 0.03                | 0.61       |
| (1,890)  | 1:41:A:VAL:H    | 1:42:A:ALA:HB3   | 10                  | 0.6      | 0.03                | 0.61       |
| (1,890)  | 1:41:A:VAL:H    | 1:42:A:ALA:HB1   | 10                  | 0.6      | 0.03                | 0.61       |
| (1,488)  | 1:59:A:THR:HG23 | 1:62:A:GLN:H     | 10                  | 0.59     | 0.02                | 0.6        |
| (1,488)  | 1:59:A:THR:HG21 | 1:62:A:GLN:H     | 10                  | 0.59     | 0.02                | 0.6        |
| (1,488)  | 1:59:A:THR:HG22 | 1:62:A:GLN:H     | 10                  | 0.59     | 0.02                | 0.6        |
| (1,744)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB3   | 10                  | 0.59     | 0.37                | 0.6        |
| (1,630)  | 1:32:A:ASP:HB3  | 1:31:A:ALA:HB1   | 10                  | 0.57     | 0.57                | 0.29       |
| (1,630)  | 1:32:A:ASP:HB3  | 1:31:A:ALA:HB2   | 10                  | 0.57     | 0.57                | 0.29       |
| (1,630)  | 1:32:A:ASP:HB3  | 1:31:A:ALA:HB3   | 10                  | 0.57     | 0.57                | 0.29       |
| (1,1445) | 1:128:A:ASN:HA  | 1:128:A:ASN:HD22 | 10                  | 0.57     | 0.03                | 0.58       |
| (1,1445) | 1:128:A:ASN:HA  | 1:133:A:THR:H    | 10                  | 0.57     | 0.03                | 0.58       |
| (1,1492) | 1:43:A:LEU:HD11 | 1:43:A:LEU:H     | 10                  | 0.57     | 0.08                | 0.59       |
| (1,1492) | 1:43:A:LEU:HD13 | 1:43:A:LEU:H     | 10                  | 0.57     | 0.08                | 0.59       |
| (1,1492) | 1:43:A:LEU:HD12 | 1:43:A:LEU:H     | 10                  | 0.57     | 0.08                | 0.59       |
| (1,1492) | 1:43:A:LEU:HD12 | 1:99:A:GLN:H     | 10                  | 0.57     | 0.08                | 0.59       |
| (1,1492) | 1:43:A:LEU:HD11 | 1:99:A:GLN:H     | 10                  | 0.57     | 0.08                | 0.59       |
| (1,87)   | 1:37:A:ILE:HD13 | 1:126:A:ILE:HA   | 10                  | 0.56     | 0.04                | 0.57       |
| (1,87)   | 1:37:A:ILE:HD12 | 1:126:A:ILE:HA   | 10                  | 0.56     | 0.04                | 0.57       |
| (1,87)   | 1:37:A:ILE:HD11 | 1:126:A:ILE:HA   | 10                  | 0.56     | 0.04                | 0.57       |
| (1,1291) | 1:45:A:SER:H    | 1:47:A:LEU:HD11  | 10                  | 0.56     | 0.03                | 0.56       |
| (1,1291) | 1:45:A:SER:H    | 1:47:A:LEU:HD12  | 10                  | 0.56     | 0.03                | 0.56       |
| (1,1291) | 1:45:A:SER:H    | 1:47:A:LEU:HD13  | 10                  | 0.56     | 0.03                | 0.56       |
| (1,1491) | 1:43:A:LEU:HD12 | 1:39:A:ASP:HA    | 10                  | 0.56     | 0.04                | 0.55       |
| (1,1491) | 1:43:A:LEU:HD11 | 1:39:A:ASP:HA    | 10                  | 0.56     | 0.04                | 0.55       |
| (1,1491) | 1:43:A:LEU:HD13 | 1:39:A:ASP:HA    | 10                  | 0.56     | 0.04                | 0.55       |
| (1,727)  | 1:107:A:GLY:HA3 | 1:108:A:LYS:HB2  | 10                  | 0.56     | 0.23                | 0.45       |
| (1,727)  | 1:107:A:GLY:HA3 | 1:108:A:LYS:HB3  | 10                  | 0.56     | 0.23                | 0.45       |
| (1,151)  | 1:38:A:SER:HB2  | 1:90:A:PRO:HB2   | 10                  | 0.55     | 0.23                | 0.55       |
| (1,151)  | 1:38:A:SER:HB2  | 1:90:A:PRO:HB3   | 10                  | 0.55     | 0.23                | 0.55       |
| (1,1318) | 1:42:A:ALA:H    | 1:88:A:ARG:HD2   | 10                  | 0.54     | 0.15                | 0.59       |
| (1,1318) | 1:42:A:ALA:H    | 1:88:A:ARG:HD3   | 10                  | 0.54     | 0.15                | 0.59       |
| (1,2)    | 1:80:A:TYR:HB3  | 1:85:A:TYR:HD1   | 10                  | 0.53     | 0.11                | 0.55       |
| (1,2)    | 1:80:A:TYR:HB3  | 1:85:A:TYR:HD2   | 10                  | 0.53     | 0.11                | 0.55       |
| (1,1238) | 1:34:A:GLN:H    | 1:31:A:ALA:HB3   | 10                  | 0.53     | 0.07                | 0.5        |
| (1,1238) | 1:34:A:GLN:H    | 1:31:A:ALA:HB2   | 10                  | 0.53     | 0.07                | 0.5        |
| (1,1238) | 1:34:A:GLN:H    | 1:31:A:ALA:HB1   | 10                  | 0.53     | 0.07                | 0.5        |
| (1,358)  | 1:64:A:LEU:HD22 | 1:100:A:LEU:HB3  | 10                  | 0.53     | 0.09                | 0.52       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,358)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HB3  | 10                  | 0.53     | 0.09                | 0.52       |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 10                  | 0.52     | 0.18                | 0.56       |
| (1,1147) | 1:101:A:VAL:HG21 | 1:105:A:ARG:H    | 10                  | 0.52     | 0.04                | 0.52       |
| (1,1147) | 1:101:A:VAL:HG22 | 1:105:A:ARG:H    | 10                  | 0.52     | 0.04                | 0.52       |
| (1,1147) | 1:101:A:VAL:HG23 | 1:105:A:ARG:H    | 10                  | 0.52     | 0.04                | 0.52       |
| (1,196)  | 1:111:A:VAL:HG13 | 1:44:A:GLU:HB2   | 10                  | 0.52     | 0.04                | 0.54       |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 10                  | 0.52     | 0.04                | 0.54       |
| (1,196)  | 1:111:A:VAL:HG12 | 1:44:A:GLU:HB2   | 10                  | 0.52     | 0.04                | 0.54       |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG23 | 10                  | 0.52     | 0.2                 | 0.5        |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG22 | 10                  | 0.52     | 0.2                 | 0.5        |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG21 | 10                  | 0.52     | 0.2                 | 0.5        |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 10                  | 0.52     | 0.1                 | 0.53       |
| (1,1446) | 1:31:A:ALA:HB2   | 1:30:A:LYS:HB3   | 10                  | 0.52     | 0.1                 | 0.54       |
| (1,1446) | 1:31:A:ALA:HB3   | 1:30:A:LYS:HB3   | 10                  | 0.52     | 0.1                 | 0.54       |
| (1,1446) | 1:31:A:ALA:HB1   | 1:30:A:LYS:HB3   | 10                  | 0.52     | 0.1                 | 0.54       |
| (1,1446) | 1:31:A:ALA:HB2   | 1:28:A:LYS:HB2   | 10                  | 0.52     | 0.1                 | 0.54       |
| (1,1503) | 1:89:A:LEU:HB2   | 1:88:A:ARG:HA    | 10                  | 0.51     | 0.12                | 0.54       |
| (1,1503) | 1:126:A:ILE:HB   | 1:113:A:SER:HA   | 10                  | 0.51     | 0.12                | 0.54       |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB2   | 10                  | 0.51     | 0.04                | 0.54       |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB1   | 10                  | 0.51     | 0.04                | 0.54       |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB3   | 10                  | 0.51     | 0.04                | 0.54       |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 10                  | 0.51     | 0.05                | 0.51       |
| (1,1498) | 1:57:A:TYR:HE1   | 1:47:A:LEU:HG    | 10                  | 0.51     | 0.11                | 0.5        |
| (1,1498) | 1:57:A:TYR:HE2   | 1:47:A:LEU:HG    | 10                  | 0.51     | 0.11                | 0.5        |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG11  | 10                  | 0.51     | 0.02                | 0.51       |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG13  | 10                  | 0.51     | 0.02                | 0.51       |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG12  | 10                  | 0.51     | 0.02                | 0.51       |
| (1,1340) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD22 | 10                  | 0.5      | 0.09                | 0.51       |
| (1,1340) | 1:109:A:VAL:HG11 | 1:128:A:ASN:HD22 | 10                  | 0.5      | 0.09                | 0.51       |
| (1,1340) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD22 | 10                  | 0.5      | 0.09                | 0.51       |
| (1,132)  | 1:41:A:VAL:HG23  | 1:45:A:SER:HB2   | 10                  | 0.5      | 0.05                | 0.5        |
| (1,132)  | 1:41:A:VAL:HG21  | 1:45:A:SER:HB2   | 10                  | 0.5      | 0.05                | 0.5        |
| (1,132)  | 1:41:A:VAL:HG22  | 1:45:A:SER:HB2   | 10                  | 0.5      | 0.05                | 0.5        |
| (1,1014) | 1:109:A:VAL:HG13 | 1:110:A:ASP:H    | 10                  | 0.49     | 0.07                | 0.49       |
| (1,1014) | 1:109:A:VAL:HG12 | 1:110:A:ASP:H    | 10                  | 0.49     | 0.07                | 0.49       |
| (1,1014) | 1:109:A:VAL:HG11 | 1:110:A:ASP:H    | 10                  | 0.49     | 0.07                | 0.49       |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 10                  | 0.49     | 0.07                | 0.51       |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG21 | 10                  | 0.49     | 0.1                 | 0.52       |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG23 | 10                  | 0.49     | 0.1                 | 0.52       |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG22 | 10                  | 0.49     | 0.1                 | 0.52       |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 10                  | 0.48     | 0.03                | 0.48       |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD12 | 10                  | 0.48     | 0.03                | 0.48       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD11 | 10                  | 0.48     | 0.03                | 0.48       |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 10                  | 0.48     | 0.01                | 0.48       |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG23  | 10                  | 0.48     | 0.04                | 0.48       |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG22  | 10                  | 0.48     | 0.04                | 0.48       |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG21  | 10                  | 0.48     | 0.04                | 0.48       |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB2   | 10                  | 0.48     | 0.09                | 0.47       |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 10                  | 0.48     | 0.09                | 0.47       |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE1   | 10                  | 0.47     | 0.12                | 0.46       |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 10                  | 0.47     | 0.12                | 0.46       |
| (1,556)  | 1:93:A:PRO:HB3   | 1:32:A:ASP:HA    | 10                  | 0.46     | 0.06                | 0.45       |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 10                  | 0.46     | 0.06                | 0.45       |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB2   | 10                  | 0.45     | 0.05                | 0.46       |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB1   | 10                  | 0.45     | 0.05                | 0.46       |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB3   | 10                  | 0.45     | 0.05                | 0.46       |
| (1,1171) | 1:100:A:LEU:HD21 | 1:101:A:VAL:H    | 10                  | 0.45     | 0.07                | 0.44       |
| (1,1171) | 1:100:A:LEU:HD23 | 1:101:A:VAL:H    | 10                  | 0.45     | 0.07                | 0.44       |
| (1,1171) | 1:100:A:LEU:HD22 | 1:101:A:VAL:H    | 10                  | 0.45     | 0.07                | 0.44       |
| (1,451)  | 1:109:A:VAL:HG11 | 1:100:A:LEU:HD11 | 10                  | 0.44     | 0.13                | 0.46       |
| (1,451)  | 1:109:A:VAL:HG13 | 1:100:A:LEU:HD11 | 10                  | 0.44     | 0.13                | 0.46       |
| (1,451)  | 1:109:A:VAL:HG11 | 1:100:A:LEU:HD13 | 10                  | 0.44     | 0.13                | 0.46       |
| (1,451)  | 1:109:A:VAL:HG12 | 1:100:A:LEU:HD11 | 10                  | 0.44     | 0.13                | 0.46       |
| (1,451)  | 1:109:A:VAL:HG11 | 1:100:A:LEU:HD12 | 10                  | 0.44     | 0.13                | 0.46       |
| (1,451)  | 1:109:A:VAL:HG12 | 1:100:A:LEU:HD12 | 10                  | 0.44     | 0.13                | 0.46       |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 10                  | 0.44     | 0.15                | 0.44       |
| (1,360)  | 1:64:A:LEU:HD12  | 1:68:A:VAL:H     | 10                  | 0.44     | 0.1                 | 0.42       |
| (1,360)  | 1:64:A:LEU:HD11  | 1:68:A:VAL:H     | 10                  | 0.44     | 0.1                 | 0.42       |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD11  | 10                  | 0.44     | 0.06                | 0.42       |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD13  | 10                  | 0.44     | 0.06                | 0.42       |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD12  | 10                  | 0.44     | 0.06                | 0.42       |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 10                  | 0.44     | 0.02                | 0.43       |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 10                  | 0.42     | 0.11                | 0.4        |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 10                  | 0.41     | 0.02                | 0.4        |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG12 | 10                  | 0.4      | 0.02                | 0.4        |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 10                  | 0.4      | 0.02                | 0.4        |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG11 | 10                  | 0.4      | 0.02                | 0.4        |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 10                  | 0.39     | 0.13                | 0.37       |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG3   | 10                  | 0.39     | 0.13                | 0.37       |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB2   | 10                  | 0.39     | 0.06                | 0.4        |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB1   | 10                  | 0.39     | 0.06                | 0.4        |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB3   | 10                  | 0.39     | 0.06                | 0.4        |
| (1,336)  | 1:52:A:LEU:HD22  | 1:48:A:ASP:HB3   | 10                  | 0.39     | 0.39                | 0.26       |
| (1,336)  | 1:52:A:LEU:HD21  | 1:48:A:ASP:HB3   | 10                  | 0.39     | 0.39                | 0.26       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,336)  | 1:52:A:LEU:HD13  | 1:48:A:ASP:HB3  | 10                  | 0.39     | 0.39                | 0.26       |
| (1,336)  | 1:52:A:LEU:HD23  | 1:48:A:ASP:HB3  | 10                  | 0.39     | 0.39                | 0.26       |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H    | 10                  | 0.39     | 0.07                | 0.38       |
| (1,512)  | 1:91:A:GLN:HB2   | 1:92:A:ASP:H    | 10                  | 0.39     | 0.07                | 0.38       |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB1  | 10                  | 0.39     | 0.02                | 0.38       |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB3  | 10                  | 0.39     | 0.02                | 0.38       |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB2  | 10                  | 0.39     | 0.02                | 0.38       |
| (1,134)  | 1:122:A:THR:HG23 | 1:123:A:ASP:H   | 10                  | 0.39     | 0.09                | 0.39       |
| (1,134)  | 1:122:A:THR:HG22 | 1:123:A:ASP:H   | 10                  | 0.39     | 0.09                | 0.39       |
| (1,134)  | 1:122:A:THR:HG21 | 1:123:A:ASP:H   | 10                  | 0.39     | 0.09                | 0.39       |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2 | 10                  | 0.38     | 0.16                | 0.32       |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB2  | 10                  | 0.38     | 0.07                | 0.4        |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB1  | 10                  | 0.38     | 0.07                | 0.4        |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB3  | 10                  | 0.38     | 0.07                | 0.4        |
| (1,4)    | 1:126:A:ILE:HG21 | 1:126:A:ILE:H   | 10                  | 0.38     | 0.09                | 0.44       |
| (1,4)    | 1:126:A:ILE:HG22 | 1:126:A:ILE:H   | 10                  | 0.38     | 0.09                | 0.44       |
| (1,4)    | 1:126:A:ILE:HG23 | 1:126:A:ILE:H   | 10                  | 0.38     | 0.09                | 0.44       |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3  | 10                  | 0.38     | 0.06                | 0.38       |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3  | 10                  | 0.38     | 0.04                | 0.38       |
| (1,1062) | 1:100:A:LEU:HD22 | 1:64:A:LEU:H    | 10                  | 0.37     | 0.03                | 0.38       |
| (1,1062) | 1:100:A:LEU:HD21 | 1:64:A:LEU:H    | 10                  | 0.37     | 0.03                | 0.38       |
| (1,1062) | 1:100:A:LEU:HD23 | 1:64:A:LEU:H    | 10                  | 0.37     | 0.03                | 0.38       |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H    | 10                  | 0.37     | 0.09                | 0.38       |
| (1,664)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HA  | 10                  | 0.37     | 0.04                | 0.37       |
| (1,664)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HA  | 10                  | 0.37     | 0.04                | 0.37       |
| (1,664)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HA  | 10                  | 0.37     | 0.04                | 0.37       |
| (1,1245) | 1:40:A:ILE:HD13  | 1:37:A:ILE:H    | 10                  | 0.37     | 0.04                | 0.36       |
| (1,1245) | 1:40:A:ILE:HD11  | 1:37:A:ILE:H    | 10                  | 0.37     | 0.04                | 0.36       |
| (1,1245) | 1:40:A:ILE:HD12  | 1:37:A:ILE:H    | 10                  | 0.37     | 0.04                | 0.36       |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD12 | 10                  | 0.36     | 0.05                | 0.37       |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD11 | 10                  | 0.36     | 0.05                | 0.37       |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD13 | 10                  | 0.36     | 0.05                | 0.37       |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H    | 10                  | 0.36     | 0.09                | 0.36       |
| (1,199)  | 1:111:A:VAL:HG12 | 1:112:A:PHE:H   | 10                  | 0.36     | 0.04                | 0.36       |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H   | 10                  | 0.36     | 0.04                | 0.36       |
| (1,199)  | 1:111:A:VAL:HG11 | 1:112:A:PHE:H   | 10                  | 0.36     | 0.04                | 0.36       |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD13 | 10                  | 0.36     | 0.09                | 0.36       |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD11 | 10                  | 0.36     | 0.09                | 0.36       |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD12 | 10                  | 0.36     | 0.09                | 0.36       |
| (1,616)  | 1:100:A:LEU:HD23 | 1:58:A:PRO:HG2  | 10                  | 0.35     | 0.04                | 0.34       |
| (1,616)  | 1:100:A:LEU:HD22 | 1:58:A:PRO:HG2  | 10                  | 0.35     | 0.04                | 0.34       |
| (1,616)  | 1:100:A:LEU:HD21 | 1:58:A:PRO:HG2  | 10                  | 0.35     | 0.04                | 0.34       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,258)  | 1:76:A:GLU:HB3   | 1:72:A:THR:HA    | 10                  | 0.35     | 0.04                | 0.37       |
| (1,258)  | 1:76:A:GLU:HB2   | 1:72:A:THR:HA    | 10                  | 0.35     | 0.04                | 0.37       |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 10                  | 0.35     | 0.02                | 0.34       |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB3   | 10                  | 0.35     | 0.05                | 0.34       |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB1   | 10                  | 0.35     | 0.05                | 0.34       |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB2   | 10                  | 0.35     | 0.05                | 0.34       |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 10                  | 0.34     | 0.09                | 0.34       |
| (1,803)  | 1:46:A:ALA:HB2   | 1:67:A:LEU:HA    | 10                  | 0.34     | 0.09                | 0.34       |
| (1,803)  | 1:46:A:ALA:HB3   | 1:67:A:LEU:HA    | 10                  | 0.34     | 0.09                | 0.34       |
| (1,803)  | 1:46:A:ALA:HB1   | 1:67:A:LEU:HA    | 10                  | 0.34     | 0.09                | 0.34       |
| (1,676)  | 1:109:A:VAL:HG23 | 1:100:A:LEU:HA   | 10                  | 0.34     | 0.06                | 0.33       |
| (1,676)  | 1:109:A:VAL:HG22 | 1:100:A:LEU:HA   | 10                  | 0.34     | 0.06                | 0.33       |
| (1,676)  | 1:109:A:VAL:HG21 | 1:100:A:LEU:HA   | 10                  | 0.34     | 0.06                | 0.33       |
| (1,1261) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD21 | 10                  | 0.34     | 0.11                | 0.34       |
| (1,1261) | 1:109:A:VAL:HG11 | 1:128:A:ASN:HD21 | 10                  | 0.34     | 0.11                | 0.34       |
| (1,1261) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD21 | 10                  | 0.34     | 0.11                | 0.34       |
| (1,484)  | 1:59:A:THR:HG23  | 1:62:A:GLN:HG2   | 10                  | 0.33     | 0.05                | 0.33       |
| (1,484)  | 1:59:A:THR:HG21  | 1:62:A:GLN:HG2   | 10                  | 0.33     | 0.05                | 0.33       |
| (1,484)  | 1:59:A:THR:HG22  | 1:62:A:GLN:HG2   | 10                  | 0.33     | 0.05                | 0.33       |
| (1,618)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:H    | 10                  | 0.33     | 0.05                | 0.34       |
| (1,618)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:H    | 10                  | 0.33     | 0.05                | 0.34       |
| (1,618)  | 1:100:A:LEU:HD23 | 1:100:A:LEU:H    | 10                  | 0.33     | 0.05                | 0.34       |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG12 | 10                  | 0.33     | 0.02                | 0.32       |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 10                  | 0.33     | 0.02                | 0.32       |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG11 | 10                  | 0.33     | 0.02                | 0.32       |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 10                  | 0.32     | 0.05                | 0.32       |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 10                  | 0.32     | 0.07                | 0.31       |
| (1,95)   | 1:37:A:ILE:HG23  | 1:41:A:VAL:H     | 10                  | 0.31     | 0.03                | 0.32       |
| (1,95)   | 1:37:A:ILE:HG22  | 1:41:A:VAL:H     | 10                  | 0.31     | 0.03                | 0.32       |
| (1,95)   | 1:37:A:ILE:HG21  | 1:41:A:VAL:H     | 10                  | 0.31     | 0.03                | 0.32       |
| (1,659)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HA    | 10                  | 0.31     | 0.04                | 0.3        |
| (1,659)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HA    | 10                  | 0.31     | 0.04                | 0.3        |
| (1,659)  | 1:111:A:VAL:HG21 | 1:40:A:ILE:HA    | 10                  | 0.31     | 0.04                | 0.3        |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 10                  | 0.31     | 0.09                | 0.29       |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 10                  | 0.3      | 0.05                | 0.29       |
| (1,201)  | 1:111:A:VAL:HG11 | 1:128:A:ASN:HD21 | 10                  | 0.3      | 0.03                | 0.32       |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 10                  | 0.3      | 0.03                | 0.32       |
| (1,201)  | 1:111:A:VAL:HG13 | 1:128:A:ASN:HD21 | 10                  | 0.3      | 0.03                | 0.32       |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 10                  | 0.3      | 0.01                | 0.3        |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 10                  | 0.3      | 0.04                | 0.3        |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB3   | 10                  | 0.29     | 0.05                | 0.28       |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB2   | 10                  | 0.29     | 0.05                | 0.28       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB1  | 10                  | 0.29     | 0.05                | 0.28       |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG22 | 10                  | 0.29     | 0.04                | 0.29       |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG21 | 10                  | 0.29     | 0.04                | 0.29       |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG23 | 10                  | 0.29     | 0.04                | 0.29       |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3 | 10                  | 0.28     | 0.05                | 0.3        |
| (1,767)  | 1:122:A:THR:HG22 | 1:121:A:ASP:H   | 10                  | 0.28     | 0.06                | 0.3        |
| (1,767)  | 1:122:A:THR:HG21 | 1:121:A:ASP:H   | 10                  | 0.28     | 0.06                | 0.3        |
| (1,767)  | 1:122:A:THR:HG23 | 1:121:A:ASP:H   | 10                  | 0.28     | 0.06                | 0.3        |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2 | 10                  | 0.28     | 0.07                | 0.26       |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA3 | 10                  | 0.28     | 0.07                | 0.26       |
| (1,779)  | 1:40:A:ILE:HG21  | 1:112:A:PHE:HA  | 10                  | 0.28     | 0.08                | 0.25       |
| (1,779)  | 1:40:A:ILE:HG23  | 1:112:A:PHE:HA  | 10                  | 0.28     | 0.08                | 0.25       |
| (1,779)  | 1:40:A:ILE:HG22  | 1:112:A:PHE:HA  | 10                  | 0.28     | 0.08                | 0.25       |
| (1,998)  | 1:43:A:LEU:HD11  | 1:43:A:LEU:H    | 10                  | 0.28     | 0.01                | 0.27       |
| (1,998)  | 1:43:A:LEU:HD13  | 1:43:A:LEU:H    | 10                  | 0.28     | 0.01                | 0.27       |
| (1,998)  | 1:43:A:LEU:HD12  | 1:43:A:LEU:H    | 10                  | 0.28     | 0.01                | 0.27       |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD1  | 10                  | 0.27     | 0.11                | 0.28       |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2  | 10                  | 0.27     | 0.11                | 0.28       |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG21 | 10                  | 0.27     | 0.01                | 0.26       |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG23 | 10                  | 0.27     | 0.01                | 0.26       |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG22 | 10                  | 0.27     | 0.01                | 0.26       |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG   | 10                  | 0.27     | 0.01                | 0.27       |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H    | 10                  | 0.27     | 0.04                | 0.26       |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2  | 10                  | 0.26     | 0.03                | 0.26       |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3  | 10                  | 0.26     | 0.03                | 0.26       |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H   | 10                  | 0.26     | 0.02                | 0.26       |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2  | 10                  | 0.25     | 0.05                | 0.25       |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG23 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG22 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG21 | 10                  | 0.25     | 0.03                | 0.24       |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA  | 10                  | 0.25     | 0.03                | 0.24       |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB3  | 10                  | 0.24     | 0.01                | 0.24       |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB1  | 10                  | 0.24     | 0.01                | 0.24       |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB2  | 10                  | 0.24     | 0.01                | 0.24       |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD1  | 10                  | 0.24     | 0.03                | 0.24       |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD2  | 10                  | 0.24     | 0.03                | 0.24       |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H    | 10                  | 0.24     | 0.03                | 0.23       |
| (1,920)  | 1:87:A:ARG:HB3   | 1:88:A:ARG:H    | 10                  | 0.24     | 0.03                | 0.23       |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H    | 10                  | 0.23     | 0.03                | 0.23       |
| (1,300)  | 1:73:A:THR:HG22  | 1:71:A:PRO:HB3  | 10                  | 0.23     | 0.05                | 0.24       |
| (1,300)  | 1:73:A:THR:HG23  | 1:71:A:PRO:HB3  | 10                  | 0.23     | 0.05                | 0.24       |
| (1,300)  | 1:73:A:THR:HG21  | 1:71:A:PRO:HB3  | 10                  | 0.23     | 0.05                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,658)  | 1:111:A:VAL:HG22 | 1:44:A:GLU:HA    | 10                  | 0.23     | 0.02                | 0.22       |
| (1,658)  | 1:111:A:VAL:HG21 | 1:44:A:GLU:HA    | 10                  | 0.23     | 0.02                | 0.22       |
| (1,658)  | 1:111:A:VAL:HG23 | 1:44:A:GLU:HA    | 10                  | 0.23     | 0.02                | 0.22       |
| (1,670)  | 1:111:A:VAL:HG11 | 1:109:A:VAL:HG23 | 10                  | 0.23     | 0.03                | 0.22       |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG23 | 10                  | 0.23     | 0.03                | 0.22       |
| (1,670)  | 1:111:A:VAL:HG13 | 1:109:A:VAL:HG22 | 10                  | 0.23     | 0.03                | 0.22       |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG21 | 10                  | 0.23     | 0.03                | 0.22       |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG22 | 10                  | 0.23     | 0.03                | 0.22       |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 10                  | 0.23     | 0.06                | 0.22       |
| (1,657)  | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD11  | 10                  | 0.22     | 0.08                | 0.21       |
| (1,657)  | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD13  | 10                  | 0.22     | 0.08                | 0.21       |
| (1,657)  | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD12  | 10                  | 0.22     | 0.08                | 0.21       |
| (1,657)  | 1:111:A:VAL:HG21 | 1:43:A:LEU:HD13  | 10                  | 0.22     | 0.08                | 0.21       |
| (1,657)  | 1:111:A:VAL:HG23 | 1:43:A:LEU:HD13  | 10                  | 0.22     | 0.08                | 0.21       |
| (1,657)  | 1:111:A:VAL:HG23 | 1:43:A:LEU:HD12  | 10                  | 0.22     | 0.08                | 0.21       |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 10                  | 0.22     | 0.01                | 0.22       |
| (1,1479) | 1:52:A:LEU:HG    | 1:49:A:MET:HA    | 10                  | 0.22     | 0.06                | 0.2        |
| (1,387)  | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 10                  | 0.22     | 0.05                | 0.22       |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 10                  | 0.22     | 0.01                | 0.22       |
| (1,228)  | 1:63:A:GLY:HA2   | 1:100:A:LEU:HB2  | 10                  | 0.21     | 0.08                | 0.18       |
| (1,904)  | 1:106:A:HIS:HB3  | 1:107:A:GLY:H    | 10                  | 0.21     | 0.07                | 0.18       |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 10                  | 0.21     | 0.03                | 0.2        |
| (1,696)  | 1:100:A:LEU:HD12 | 1:100:A:LEU:HA   | 10                  | 0.21     | 0.03                | 0.2        |
| (1,696)  | 1:100:A:LEU:HD11 | 1:100:A:LEU:HA   | 10                  | 0.21     | 0.03                | 0.2        |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 10                  | 0.21     | 0.02                | 0.2        |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE1  | 10                  | 0.21     | 0.02                | 0.2        |
| (1,1516) | 1:49:A:MET:HB3   | 1:49:A:MET:H     | 10                  | 0.2      | 0.01                | 0.2        |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 10                  | 0.2      | 0.01                | 0.2        |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG2   | 10                  | 0.2      | 0.01                | 0.2        |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG12 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG13 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG11 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,1041) | 1:100:A:LEU:HB2  | 1:100:A:LEU:H    | 10                  | 0.2      | 0.05                | 0.19       |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG21  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG22  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG23  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,21)   | 1:31:A:ALA:HA    | 1:30:A:LYS:HB3   | 10                  | 0.2      | 0.03                | 0.2        |
| (1,282)  | 1:78:A:ARG:HD2   | 1:78:A:ARG:HG3   | 10                  | 0.2      | 0.03                | 0.19       |
| (1,282)  | 1:78:A:ARG:HD3   | 1:78:A:ARG:HG2   | 10                  | 0.2      | 0.03                | 0.19       |
| (1,282)  | 1:78:A:ARG:HD2   | 1:78:A:ARG:HG2   | 10                  | 0.2      | 0.03                | 0.19       |
| (1,282)  | 1:78:A:ARG:HD3   | 1:78:A:ARG:HG3   | 10                  | 0.2      | 0.03                | 0.19       |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 10                  | 0.19     | 0.01                | 0.2        |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1411) | 1:66:A:ALA:HB3   | 1:68:A:VAL:H    | 10                  | 0.19     | 0.03                | 0.2        |
| (1,1411) | 1:66:A:ALA:HB2   | 1:68:A:VAL:H    | 10                  | 0.19     | 0.03                | 0.2        |
| (1,1411) | 1:66:A:ALA:HB1   | 1:68:A:VAL:H    | 10                  | 0.19     | 0.03                | 0.2        |
| (1,255)  | 1:43:A:LEU:HB3   | 1:40:A:ILE:HA   | 10                  | 0.19     | 0.02                | 0.18       |
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H   | 10                  | 0.19     | 0.05                | 0.18       |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2  | 10                  | 0.19     | 0.09                | 0.16       |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD21 | 10                  | 0.19     | 0.06                | 0.2        |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD23 | 10                  | 0.19     | 0.06                | 0.2        |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD22 | 10                  | 0.19     | 0.06                | 0.2        |
| (1,435)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:H    | 10                  | 0.19     | 0.03                | 0.19       |
| (1,435)  | 1:41:A:VAL:HG13  | 1:42:A:ALA:H    | 10                  | 0.19     | 0.03                | 0.19       |
| (1,435)  | 1:41:A:VAL:HG12  | 1:42:A:ALA:H    | 10                  | 0.19     | 0.03                | 0.19       |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2  | 10                  | 0.18     | 0.07                | 0.17       |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD1  | 10                  | 0.18     | 0.07                | 0.17       |
| (1,726)  | 1:101:A:VAL:HB   | 1:100:A:LEU:HA  | 10                  | 0.18     | 0.02                | 0.18       |
| (1,85)   | 1:37:A:ILE:HA    | 1:40:A:ILE:HD13 | 10                  | 0.17     | 0.02                | 0.17       |
| (1,85)   | 1:37:A:ILE:HA    | 1:40:A:ILE:HD11 | 10                  | 0.17     | 0.02                | 0.17       |
| (1,85)   | 1:37:A:ILE:HA    | 1:40:A:ILE:HD12 | 10                  | 0.17     | 0.02                | 0.17       |
| (1,355)  | 1:131:A:VAL:HB   | 1:131:A:VAL:H   | 10                  | 0.17     | 0.01                | 0.17       |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG11 | 10                  | 0.17     | 0.02                | 0.18       |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG13 | 10                  | 0.17     | 0.02                | 0.18       |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG12 | 10                  | 0.17     | 0.02                | 0.18       |
| (1,165)  | 1:30:A:LYS:HA    | 1:30:A:LYS:HB2  | 10                  | 0.17     | 0.05                | 0.15       |
| (1,927)  | 1:49:A:MET:HB3   | 1:49:A:MET:H    | 10                  | 0.16     | 0.01                | 0.16       |
| (1,270)  | 1:85:A:TYR:HA    | 1:81:A:PRO:HB2  | 10                  | 0.16     | 0.02                | 0.16       |
| (1,10)   | 1:28:A:LYS:HE3   | 1:28:A:LYS:HD3  | 10                  | 0.16     | 0.03                | 0.16       |
| (1,10)   | 1:28:A:LYS:HE2   | 1:28:A:LYS:HD3  | 10                  | 0.16     | 0.03                | 0.16       |
| (1,10)   | 1:28:A:LYS:HE2   | 1:28:A:LYS:HD2  | 10                  | 0.16     | 0.03                | 0.16       |
| (1,10)   | 1:28:A:LYS:HE3   | 1:28:A:LYS:HD2  | 10                  | 0.16     | 0.03                | 0.16       |
| (1,922)  | 1:86:A:ILE:HD11  | 1:88:A:ARG:H    | 10                  | 0.14     | 0.04                | 0.14       |
| (1,922)  | 1:86:A:ILE:HD13  | 1:88:A:ARG:H    | 10                  | 0.14     | 0.04                | 0.14       |
| (1,922)  | 1:86:A:ILE:HD12  | 1:88:A:ARG:H    | 10                  | 0.14     | 0.04                | 0.14       |
| (1,350)  | 1:112:A:PHE:HA   | 1:112:A:PHE:HD1 | 10                  | 0.14     | 0.03                | 0.13       |
| (1,350)  | 1:112:A:PHE:HA   | 1:112:A:PHE:HD2 | 10                  | 0.14     | 0.03                | 0.13       |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG21 | 10                  | 0.14     | 0.02                | 0.13       |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG22 | 10                  | 0.14     | 0.02                | 0.13       |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG23 | 10                  | 0.14     | 0.02                | 0.13       |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H    | 10                  | 0.13     | 0.0                 | 0.13       |
| (1,689)  | 1:111:A:VAL:HB   | 1:111:A:VAL:H   | 10                  | 0.12     | 0.01                | 0.11       |
| (1,492)  | 1:122:A:THR:HG21 | 1:119:A:MET:HG2 | 9                   | 1.13     | 0.11                | 1.11       |
| (1,492)  | 1:122:A:THR:HG23 | 1:119:A:MET:HG2 | 9                   | 1.13     | 0.11                | 1.11       |
| (1,492)  | 1:122:A:THR:HG22 | 1:119:A:MET:HG2 | 9                   | 1.13     | 0.11                | 1.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE1   | 9                   | 1.08     | 0.3                 | 1.06       |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE2   | 9                   | 1.08     | 0.3                 | 1.06       |
| (1,1522) | 1:105:A:ARG:HD2  | 1:102:A:SER:HA   | 9                   | 0.94     | 0.28                | 0.96       |
| (1,1522) | 1:105:A:ARG:HD3  | 1:106:A:HIS:HA   | 9                   | 0.94     | 0.28                | 0.96       |
| (1,1522) | 1:105:A:ARG:HD2  | 1:106:A:HIS:HA   | 9                   | 0.94     | 0.28                | 0.96       |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 9                   | 0.73     | 0.08                | 0.7        |
| (1,93)   | 1:37:A:ILE:HG22  | 1:132:A:GLY:HA2  | 9                   | 0.63     | 0.05                | 0.64       |
| (1,93)   | 1:37:A:ILE:HG21  | 1:132:A:GLY:HA2  | 9                   | 0.63     | 0.05                | 0.64       |
| (1,93)   | 1:37:A:ILE:HG23  | 1:132:A:GLY:HA2  | 9                   | 0.63     | 0.05                | 0.64       |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 9                   | 0.55     | 0.03                | 0.54       |
| (1,1444) | 1:27:A:ASN:HB3   | 1:30:A:LYS:HB3   | 9                   | 0.5      | 0.29                | 0.37       |
| (1,1444) | 1:27:A:ASN:HB2   | 1:28:A:LYS:HB2   | 9                   | 0.5      | 0.29                | 0.37       |
| (1,1444) | 1:27:A:ASN:HB3   | 1:28:A:LYS:HB2   | 9                   | 0.5      | 0.29                | 0.37       |
| (1,1444) | 1:27:A:ASN:HB2   | 1:30:A:LYS:HB3   | 9                   | 0.5      | 0.29                | 0.37       |
| (1,966)  | 1:96:A:ALA:H     | 1:94:A:TRP:HZ3   | 9                   | 0.48     | 0.58                | 0.17       |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD23  | 9                   | 0.46     | 0.1                 | 0.4        |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD22  | 9                   | 0.46     | 0.1                 | 0.4        |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD21  | 9                   | 0.46     | 0.1                 | 0.4        |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD2   | 9                   | 0.45     | 0.09                | 0.47       |
| (1,1537) | 1:49:A:MET:H     | 1:136:A:HIS:HD2  | 9                   | 0.45     | 0.09                | 0.47       |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD1   | 9                   | 0.45     | 0.09                | 0.47       |
| (1,1523) | 1:140:A:SER:HB2  | 1:139:A:GLY:H    | 9                   | 0.44     | 0.13                | 0.5        |
| (1,1523) | 1:140:A:SER:HB3  | 1:139:A:GLY:H    | 9                   | 0.44     | 0.13                | 0.5        |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 9                   | 0.43     | 0.1                 | 0.48       |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD2   | 9                   | 0.43     | 0.1                 | 0.48       |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 9                   | 0.41     | 0.15                | 0.36       |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 9                   | 0.39     | 0.11                | 0.43       |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 9                   | 0.36     | 0.02                | 0.35       |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG22 | 9                   | 0.35     | 0.1                 | 0.41       |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG23 | 9                   | 0.35     | 0.1                 | 0.41       |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG21 | 9                   | 0.35     | 0.1                 | 0.41       |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 9                   | 0.35     | 0.11                | 0.35       |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG2   | 9                   | 0.35     | 0.03                | 0.36       |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG3   | 9                   | 0.35     | 0.03                | 0.36       |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD13  | 9                   | 0.33     | 0.11                | 0.26       |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD12  | 9                   | 0.33     | 0.11                | 0.26       |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD11  | 9                   | 0.33     | 0.11                | 0.26       |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 9                   | 0.3      | 0.0                 | 0.3        |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 9                   | 0.29     | 0.09                | 0.3        |
| (1,1350) | 1:54:A:ASN:HB2   | 1:52:A:LEU:H     | 9                   | 0.29     | 0.09                | 0.3        |
| (1,738)  | 1:78:A:ARG:HD2   | 1:54:A:ASN:H     | 9                   | 0.28     | 0.1                 | 0.25       |
| (1,738)  | 1:78:A:ARG:HD3   | 1:54:A:ASN:H     | 9                   | 0.28     | 0.1                 | 0.25       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 9                   | 0.28     | 0.12                | 0.25       |
| (1,1462) | 1:45:A:SER:HB2   | 1:44:A:GLU:HB3   | 9                   | 0.27     | 0.1                 | 0.25       |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB2   | 9                   | 0.24     | 0.07                | 0.2        |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB3   | 9                   | 0.24     | 0.07                | 0.2        |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB1   | 9                   | 0.24     | 0.07                | 0.2        |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 9                   | 0.24     | 0.11                | 0.21       |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 9                   | 0.23     | 0.03                | 0.24       |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG3   | 9                   | 0.22     | 0.06                | 0.24       |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG2   | 9                   | 0.22     | 0.06                | 0.24       |
| (1,298)  | 1:101:A:VAL:HG12 | 1:110:A:ASP:HB2  | 9                   | 0.21     | 0.08                | 0.22       |
| (1,298)  | 1:101:A:VAL:HG13 | 1:110:A:ASP:HB2  | 9                   | 0.21     | 0.08                | 0.22       |
| (1,298)  | 1:101:A:VAL:HG11 | 1:110:A:ASP:HB2  | 9                   | 0.21     | 0.08                | 0.22       |
| (1,136)  | 1:50:A:TYR:HA    | 1:54:A:ASN:HB2   | 9                   | 0.2      | 0.08                | 0.16       |
| (1,136)  | 1:50:A:TYR:HA    | 1:54:A:ASN:HB3   | 9                   | 0.2      | 0.08                | 0.16       |
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG23  | 9                   | 0.2      | 0.07                | 0.19       |
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG22  | 9                   | 0.2      | 0.07                | 0.19       |
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG21  | 9                   | 0.2      | 0.07                | 0.19       |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG13 | 9                   | 0.18     | 0.07                | 0.15       |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG12 | 9                   | 0.18     | 0.07                | 0.15       |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG11 | 9                   | 0.18     | 0.07                | 0.15       |
| (1,552)  | 1:85:A:TYR:HB3   | 1:67:A:LEU:HA    | 9                   | 0.15     | 0.03                | 0.15       |
| (1,54)   | 1:28:A:LYS:HD2   | 1:28:A:LYS:HG3   | 9                   | 0.15     | 0.02                | 0.14       |
| (1,54)   | 1:28:A:LYS:HD3   | 1:28:A:LYS:HG2   | 9                   | 0.15     | 0.02                | 0.14       |
| (1,54)   | 1:28:A:LYS:HD2   | 1:28:A:LYS:HG2   | 9                   | 0.15     | 0.02                | 0.14       |
| (1,75)   | 1:35:A:LYS:HG3   | 1:35:A:LYS:HD2   | 9                   | 0.15     | 0.01                | 0.15       |
| (1,75)   | 1:35:A:LYS:HG2   | 1:35:A:LYS:HD3   | 9                   | 0.15     | 0.01                | 0.15       |
| (1,822)  | 1:76:A:GLU:HB3   | 1:76:A:GLU:H     | 9                   | 0.14     | 0.02                | 0.14       |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG23  | 9                   | 0.13     | 0.02                | 0.13       |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG21  | 9                   | 0.13     | 0.02                | 0.13       |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG22  | 9                   | 0.13     | 0.02                | 0.13       |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB3   | 9                   | 0.12     | 0.01                | 0.11       |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB1   | 9                   | 0.12     | 0.01                | 0.11       |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB2   | 9                   | 0.12     | 0.01                | 0.11       |
| (1,655)  | 1:56:A:ARG:HB3   | 1:57:A:TYR:H     | 8                   | 0.48     | 0.25                | 0.51       |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG23  | 8                   | 0.47     | 0.29                | 0.37       |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG21  | 8                   | 0.47     | 0.29                | 0.37       |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG22  | 8                   | 0.47     | 0.29                | 0.37       |
| (1,1562) | 1:102:A:SER:H    | 1:109:A:VAL:HB   | 8                   | 0.47     | 0.29                | 0.37       |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD2   | 8                   | 0.47     | 0.14                | 0.5        |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD3   | 8                   | 0.47     | 0.14                | 0.5        |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 8                   | 0.44     | 0.28                | 0.26       |
| (1,335)  | 1:52:A:LEU:HD22  | 1:49:A:MET:HG2   | 8                   | 0.44     | 0.04                | 0.44       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,335)  | 1:52:A:LEU:HD21  | 1:49:A:MET:HG2   | 8                   | 0.44     | 0.04                | 0.44       |
| (1,335)  | 1:52:A:LEU:HD23  | 1:49:A:MET:HG2   | 8                   | 0.44     | 0.04                | 0.44       |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG2   | 8                   | 0.38     | 0.09                | 0.4        |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG3   | 8                   | 0.38     | 0.09                | 0.4        |
| (1,766)  | 1:131:A:VAL:HG22 | 1:128:A:ASN:HB3  | 8                   | 0.37     | 0.19                | 0.4        |
| (1,766)  | 1:131:A:VAL:HG23 | 1:128:A:ASN:HB3  | 8                   | 0.37     | 0.19                | 0.4        |
| (1,766)  | 1:131:A:VAL:HG21 | 1:128:A:ASN:HB3  | 8                   | 0.37     | 0.19                | 0.4        |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 8                   | 0.36     | 0.04                | 0.36       |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD22  | 8                   | 0.34     | 0.06                | 0.35       |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD21  | 8                   | 0.34     | 0.06                | 0.35       |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD23  | 8                   | 0.34     | 0.06                | 0.35       |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG21 | 8                   | 0.33     | 0.09                | 0.35       |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG23 | 8                   | 0.33     | 0.09                | 0.35       |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG22 | 8                   | 0.33     | 0.09                | 0.35       |
| (1,253)  | 1:92:A:ASP:HB2   | 1:113:A:SER:HB3  | 8                   | 0.29     | 0.05                | 0.29       |
| (1,253)  | 1:92:A:ASP:HB3   | 1:113:A:SER:HB3  | 8                   | 0.29     | 0.05                | 0.29       |
| (1,720)  | 1:108:A:LYS:HA   | 1:103:A:PRO:HB3  | 8                   | 0.29     | 0.14                | 0.21       |
| (1,720)  | 1:108:A:LYS:HA   | 1:103:A:PRO:HB2  | 8                   | 0.29     | 0.14                | 0.21       |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE1   | 8                   | 0.24     | 0.1                 | 0.24       |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE2   | 8                   | 0.24     | 0.1                 | 0.24       |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG23  | 8                   | 0.24     | 0.05                | 0.24       |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG21  | 8                   | 0.24     | 0.05                | 0.24       |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG22  | 8                   | 0.24     | 0.05                | 0.24       |
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 8                   | 0.24     | 0.07                | 0.22       |
| (1,1569) | 1:92:A:ASP:H     | 1:95:A:GLY:H     | 8                   | 0.22     | 0.07                | 0.2        |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD22 | 8                   | 0.21     | 0.05                | 0.2        |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD21 | 8                   | 0.21     | 0.05                | 0.2        |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD23 | 8                   | 0.21     | 0.05                | 0.2        |
| (1,1577) | 1:85:A:TYR:H     | 1:68:A:VAL:H     | 8                   | 0.2      | 0.05                | 0.18       |
| (1,337)  | 1:52:A:LEU:HD12  | 1:52:A:LEU:HB3   | 8                   | 0.2      | 0.03                | 0.2        |
| (1,337)  | 1:52:A:LEU:HD11  | 1:52:A:LEU:HB3   | 8                   | 0.2      | 0.03                | 0.2        |
| (1,337)  | 1:52:A:LEU:HD13  | 1:52:A:LEU:HB3   | 8                   | 0.2      | 0.03                | 0.2        |
| (1,474)  | 1:69:A:LYS:HB2   | 1:68:A:VAL:HB    | 8                   | 0.19     | 0.04                | 0.2        |
| (1,908)  | 1:117:A:ASP:HB2  | 1:117:A:ASP:H    | 8                   | 0.18     | 0.02                | 0.18       |
| (1,318)  | 1:124:A:ASP:HA   | 1:124:A:ASP:HB3  | 8                   | 0.18     | 0.01                | 0.18       |
| (1,784)  | 1:114:A:TYR:HA   | 1:126:A:ILE:HB   | 8                   | 0.18     | 0.03                | 0.18       |
| (1,592)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HA    | 8                   | 0.16     | 0.04                | 0.16       |
| (1,592)  | 1:88:A:ARG:HD2   | 1:88:A:ARG:HA    | 8                   | 0.16     | 0.04                | 0.16       |
| (1,483)  | 1:59:A:THR:HG23  | 1:58:A:PRO:HA    | 8                   | 0.16     | 0.02                | 0.16       |
| (1,483)  | 1:59:A:THR:HG21  | 1:58:A:PRO:HA    | 8                   | 0.16     | 0.02                | 0.16       |
| (1,483)  | 1:59:A:THR:HG22  | 1:58:A:PRO:HA    | 8                   | 0.16     | 0.02                | 0.16       |
| (1,466)  | 1:82:A:GLN:HG3   | 1:83:A:ASP:H     | 8                   | 0.15     | 0.03                | 0.15       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,466)  | 1:82:A:GLN:HG2   | 1:83:A:ASP:H     | 8                   | 0.15     | 0.03                | 0.15       |
| (1,291)  | 1:58:A:PRO:HA    | 1:62:A:GLN:HB2   | 8                   | 0.15     | 0.02                | 0.15       |
| (1,1015) | 1:104:A:GLY:H    | 1:110:A:ASP:H    | 8                   | 0.12     | 0.02                | 0.13       |
| (1,915)  | 1:122:A:THR:H    | 1:121:A:ASP:HB3  | 8                   | 0.12     | 0.04                | 0.11       |
| (1,1317) | 1:97:A:GLU:HA    | 1:91:A:GLN:HE21  | 7                   | 1.22     | 0.32                | 1.28       |
| (1,1474) | 1:56:A:ARG:HD3   | 1:50:A:TYR:HE1   | 7                   | 0.55     | 0.13                | 0.57       |
| (1,1474) | 1:56:A:ARG:HD2   | 1:50:A:TYR:HE1   | 7                   | 0.55     | 0.13                | 0.57       |
| (1,1474) | 1:56:A:ARG:HD2   | 1:50:A:TYR:HE2   | 7                   | 0.55     | 0.13                | 0.57       |
| (1,1474) | 1:56:A:ARG:HD3   | 1:50:A:TYR:HE2   | 7                   | 0.55     | 0.13                | 0.57       |
| (1,449)  | 1:109:A:VAL:HG12 | 1:108:A:LYS:HD3  | 7                   | 0.51     | 0.12                | 0.54       |
| (1,449)  | 1:109:A:VAL:HG11 | 1:108:A:LYS:HD3  | 7                   | 0.51     | 0.12                | 0.54       |
| (1,449)  | 1:109:A:VAL:HG13 | 1:108:A:LYS:HD3  | 7                   | 0.51     | 0.12                | 0.54       |
| (1,667)  | 1:109:A:VAL:HG23 | 1:108:A:LYS:HB2  | 7                   | 0.49     | 0.26                | 0.46       |
| (1,667)  | 1:109:A:VAL:HG22 | 1:108:A:LYS:HB2  | 7                   | 0.49     | 0.26                | 0.46       |
| (1,667)  | 1:109:A:VAL:HG21 | 1:108:A:LYS:HB2  | 7                   | 0.49     | 0.26                | 0.46       |
| (1,334)  | 1:52:A:LEU:HD23  | 1:51:A:LYS:HG2   | 7                   | 0.46     | 0.11                | 0.4        |
| (1,334)  | 1:52:A:LEU:HD22  | 1:51:A:LYS:HG2   | 7                   | 0.46     | 0.11                | 0.4        |
| (1,1506) | 1:66:A:ALA:HB3   | 1:71:A:PRO:HB2   | 7                   | 0.44     | 0.09                | 0.47       |
| (1,1506) | 1:66:A:ALA:HB1   | 1:71:A:PRO:HB2   | 7                   | 0.44     | 0.09                | 0.47       |
| (1,1506) | 1:66:A:ALA:HB2   | 1:71:A:PRO:HB2   | 7                   | 0.44     | 0.09                | 0.47       |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 7                   | 0.41     | 0.12                | 0.47       |
| (1,1504) | 1:96:A:ALA:HB3   | 1:95:A:GLY:H     | 7                   | 0.29     | 0.1                 | 0.29       |
| (1,1504) | 1:96:A:ALA:HB2   | 1:95:A:GLY:H     | 7                   | 0.29     | 0.1                 | 0.29       |
| (1,1504) | 1:96:A:ALA:HB1   | 1:95:A:GLY:H     | 7                   | 0.29     | 0.1                 | 0.29       |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 7                   | 0.28     | 0.04                | 0.29       |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD11  | 7                   | 0.26     | 0.07                | 0.29       |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD13  | 7                   | 0.26     | 0.07                | 0.29       |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD12  | 7                   | 0.26     | 0.07                | 0.29       |
| (1,222)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HB2   | 7                   | 0.22     | 0.06                | 0.19       |
| (1,222)  | 1:88:A:ARG:HD2   | 1:88:A:ARG:HB3   | 7                   | 0.22     | 0.06                | 0.19       |
| (1,57)   | 1:34:A:GLN:HA    | 1:37:A:ILE:H     | 7                   | 0.2      | 0.03                | 0.2        |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG22 | 7                   | 0.2      | 0.04                | 0.22       |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG21 | 7                   | 0.2      | 0.04                | 0.22       |
| (1,610)  | 1:66:A:ALA:HB3   | 1:62:A:GLN:HE21  | 7                   | 0.2      | 0.04                | 0.19       |
| (1,610)  | 1:66:A:ALA:HB2   | 1:62:A:GLN:HE21  | 7                   | 0.2      | 0.04                | 0.19       |
| (1,610)  | 1:66:A:ALA:HB1   | 1:62:A:GLN:HE21  | 7                   | 0.2      | 0.04                | 0.19       |
| (1,1248) | 1:57:A:TYR:H     | 1:57:A:TYR:HE2   | 7                   | 0.18     | 0.03                | 0.16       |
| (1,1248) | 1:57:A:TYR:H     | 1:57:A:TYR:HE1   | 7                   | 0.18     | 0.03                | 0.16       |
| (1,984)  | 1:96:A:ALA:HB1   | 1:97:A:GLU:H     | 7                   | 0.18     | 0.06                | 0.16       |
| (1,984)  | 1:96:A:ALA:HB3   | 1:97:A:GLU:H     | 7                   | 0.18     | 0.06                | 0.16       |
| (1,984)  | 1:96:A:ALA:HB2   | 1:97:A:GLU:H     | 7                   | 0.18     | 0.06                | 0.16       |
| (1,987)  | 1:117:A:ASP:H    | 1:119:A:MET:H    | 7                   | 0.16     | 0.06                | 0.14       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1563) | 1:100:A:LEU:HG   | 1:102:A:SER:H   | 7                   | 0.16     | 0.03                | 0.16       |
| (1,367)  | 1:103:A:PRO:HB3  | 1:104:A:GLY:H   | 7                   | 0.15     | 0.03                | 0.14       |
| (1,634)  | 1:79:A:SER:HB3   | 1:54:A:ASN:HA   | 6                   | 1.0      | 0.6                 | 1.28       |
| (1,632)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HG3  | 6                   | 0.96     | 0.76                | 0.73       |
| (1,632)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HG2  | 6                   | 0.96     | 0.76                | 0.73       |
| (1,1494) | 1:122:A:THR:HG22 | 1:121:A:ASP:HB3 | 6                   | 0.6      | 0.21                | 0.6        |
| (1,1494) | 1:122:A:THR:HG21 | 1:121:A:ASP:HB3 | 6                   | 0.6      | 0.21                | 0.6        |
| (1,1494) | 1:122:A:THR:HG23 | 1:121:A:ASP:HB3 | 6                   | 0.6      | 0.21                | 0.6        |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE2  | 6                   | 0.53     | 0.12                | 0.52       |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE3  | 6                   | 0.53     | 0.12                | 0.52       |
| (1,1262) | 1:134:A:SER:H    | 1:132:A:GLY:HA3 | 6                   | 0.42     | 0.16                | 0.45       |
| (1,1262) | 1:134:A:SER:H    | 1:132:A:GLY:HA2 | 6                   | 0.42     | 0.16                | 0.45       |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB3 | 6                   | 0.41     | 0.09                | 0.44       |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB2 | 6                   | 0.41     | 0.09                | 0.44       |
| (1,1176) | 1:26:A:GLY:H     | 1:24:A:GLY:HA2  | 6                   | 0.39     | 0.11                | 0.41       |
| (1,1176) | 1:26:A:GLY:H     | 1:24:A:GLY:HA3  | 6                   | 0.39     | 0.11                | 0.41       |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD2 | 6                   | 0.36     | 0.21                | 0.28       |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD1 | 6                   | 0.36     | 0.21                | 0.28       |
| (1,1575) | 1:118:A:GLY:H    | 1:114:A:TYR:HD2 | 6                   | 0.35     | 0.2                 | 0.34       |
| (1,1575) | 1:118:A:GLY:H    | 1:114:A:TYR:HD1 | 6                   | 0.35     | 0.2                 | 0.34       |
| (1,978)  | 1:98:A:TYR:HB3   | 1:98:A:TYR:H    | 6                   | 0.34     | 0.04                | 0.35       |
| (1,544)  | 1:57:A:TYR:HA    | 1:57:A:TYR:HD1  | 6                   | 0.28     | 0.07                | 0.31       |
| (1,544)  | 1:57:A:TYR:HA    | 1:57:A:TYR:HD2  | 6                   | 0.28     | 0.07                | 0.31       |
| (1,1580) | 1:48:A:ASP:H     | 1:52:A:LEU:HD22 | 6                   | 0.27     | 0.07                | 0.25       |
| (1,1580) | 1:48:A:ASP:H     | 1:52:A:LEU:HD21 | 6                   | 0.27     | 0.07                | 0.25       |
| (1,1580) | 1:48:A:ASP:H     | 1:67:A:LEU:HD12 | 6                   | 0.27     | 0.07                | 0.25       |
| (1,1580) | 1:48:A:ASP:H     | 1:67:A:LEU:HD21 | 6                   | 0.27     | 0.07                | 0.25       |
| (1,1580) | 1:48:A:ASP:H     | 1:52:A:LEU:HD13 | 6                   | 0.27     | 0.07                | 0.25       |
| (1,1457) | 1:41:A:VAL:HB    | 1:133:A:THR:H   | 6                   | 0.22     | 0.03                | 0.22       |
| (1,1481) | 1:131:A:VAL:HB   | 1:37:A:ILE:HD13 | 6                   | 0.2      | 0.05                | 0.22       |
| (1,1481) | 1:37:A:ILE:HG23  | 1:131:A:VAL:HB  | 6                   | 0.2      | 0.05                | 0.22       |
| (1,1481) | 1:37:A:ILE:HG22  | 1:131:A:VAL:HB  | 6                   | 0.2      | 0.05                | 0.22       |
| (1,1481) | 1:37:A:ILE:HG21  | 1:131:A:VAL:HB  | 6                   | 0.2      | 0.05                | 0.22       |
| (1,1091) | 1:32:A:ASP:H     | 1:28:A:LYS:HG3  | 6                   | 0.18     | 0.07                | 0.15       |
| (1,1091) | 1:32:A:ASP:H     | 1:28:A:LYS:HG2  | 6                   | 0.18     | 0.07                | 0.15       |
| (1,1452) | 1:37:A:ILE:HA    | 1:37:A:ILE:HD12 | 6                   | 0.17     | 0.05                | 0.16       |
| (1,1452) | 1:37:A:ILE:HA    | 1:37:A:ILE:HD11 | 6                   | 0.17     | 0.05                | 0.16       |
| (1,1452) | 1:37:A:ILE:HA    | 1:37:A:ILE:HD13 | 6                   | 0.17     | 0.05                | 0.16       |
| (1,595)  | 1:123:A:ASP:HA   | 1:123:A:ASP:HB3 | 6                   | 0.17     | 0.03                | 0.17       |
| (1,595)  | 1:123:A:ASP:HA   | 1:123:A:ASP:HB2 | 6                   | 0.17     | 0.03                | 0.17       |
| (1,11)   | 1:69:A:LYS:HE3   | 1:69:A:LYS:HG2  | 6                   | 0.16     | 0.03                | 0.16       |
| (1,11)   | 1:69:A:LYS:HE2   | 1:69:A:LYS:HG3  | 6                   | 0.16     | 0.03                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,11)   | 1:69:A:LYS:HE2   | 1:69:A:LYS:HG2   | 6                   | 0.16     | 0.03                | 0.16       |
| (1,852)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:H    | 6                   | 0.14     | 0.02                | 0.14       |
| (1,1218) | 1:115:A:GLY:H    | 1:114:A:TYR:HB3  | 6                   | 0.13     | 0.02                | 0.13       |
| (1,226)  | 1:60:A:THR:HA    | 1:63:A:GLY:H     | 6                   | 0.12     | 0.01                | 0.12       |
| (1,750)  | 1:53:A:ASP:HB2   | 1:85:A:TYR:HD1   | 6                   | 0.12     | 0.02                | 0.12       |
| (1,750)  | 1:53:A:ASP:HB2   | 1:85:A:TYR:HD2   | 6                   | 0.12     | 0.02                | 0.12       |
| (1,649)  | 1:42:A:ALA:HB1   | 1:43:A:LEU:H     | 6                   | 0.12     | 0.01                | 0.12       |
| (1,649)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:H     | 6                   | 0.12     | 0.01                | 0.12       |
| (1,649)  | 1:42:A:ALA:HB2   | 1:43:A:LEU:H     | 6                   | 0.12     | 0.01                | 0.12       |
| (1,666)  | 1:109:A:VAL:HG22 | 1:44:A:GLU:HG2   | 5                   | 0.83     | 0.09                | 0.86       |
| (1,666)  | 1:109:A:VAL:HG23 | 1:44:A:GLU:HG2   | 5                   | 0.83     | 0.09                | 0.86       |
| (1,666)  | 1:109:A:VAL:HG21 | 1:44:A:GLU:HG2   | 5                   | 0.83     | 0.09                | 0.86       |
| (1,826)  | 1:35:A:LYS:H     | 1:35:A:LYS:HD3   | 5                   | 0.58     | 0.06                | 0.58       |
| (1,1047) | 1:56:A:ARG:H     | 1:56:A:ARG:HG3   | 5                   | 0.56     | 0.21                | 0.65       |
| (1,1047) | 1:56:A:ARG:H     | 1:56:A:ARG:HG2   | 5                   | 0.56     | 0.21                | 0.65       |
| (1,52)   | 1:33:A:ARG:HD2   | 1:37:A:ILE:HD11  | 5                   | 0.47     | 0.1                 | 0.43       |
| (1,52)   | 1:33:A:ARG:HD3   | 1:37:A:ILE:HD13  | 5                   | 0.47     | 0.1                 | 0.43       |
| (1,52)   | 1:33:A:ARG:HD2   | 1:37:A:ILE:HD13  | 5                   | 0.47     | 0.1                 | 0.43       |
| (1,52)   | 1:33:A:ARG:HD2   | 1:37:A:ILE:HD12  | 5                   | 0.47     | 0.1                 | 0.43       |
| (1,52)   | 1:33:A:ARG:HD3   | 1:37:A:ILE:HD11  | 5                   | 0.47     | 0.1                 | 0.43       |
| (1,699)  | 1:101:A:VAL:HG22 | 1:105:A:ARG:HD2  | 5                   | 0.42     | 0.18                | 0.37       |
| (1,699)  | 1:101:A:VAL:HG23 | 1:105:A:ARG:HD2  | 5                   | 0.42     | 0.18                | 0.37       |
| (1,699)  | 1:101:A:VAL:HG23 | 1:105:A:ARG:HD3  | 5                   | 0.42     | 0.18                | 0.37       |
| (1,806)  | 1:37:A:ILE:HG21  | 1:34:A:GLN:HE22  | 5                   | 0.38     | 0.08                | 0.42       |
| (1,806)  | 1:37:A:ILE:HG22  | 1:34:A:GLN:HE22  | 5                   | 0.38     | 0.08                | 0.42       |
| (1,806)  | 1:37:A:ILE:HG23  | 1:34:A:GLN:HE22  | 5                   | 0.38     | 0.08                | 0.42       |
| (1,810)  | 1:36:A:ALA:HA    | 1:113:A:SER:HB2  | 5                   | 0.33     | 0.04                | 0.31       |
| (1,525)  | 1:61:A:GLU:HG2   | 1:73:A:THR:HG23  | 5                   | 0.29     | 0.14                | 0.24       |
| (1,525)  | 1:61:A:GLU:HG3   | 1:73:A:THR:HG23  | 5                   | 0.29     | 0.14                | 0.24       |
| (1,525)  | 1:61:A:GLU:HG2   | 1:73:A:THR:HG22  | 5                   | 0.29     | 0.14                | 0.24       |
| (1,1470) | 1:86:A:ILE:HG21  | 1:85:A:TYR:H     | 5                   | 0.29     | 0.08                | 0.31       |
| (1,1470) | 1:86:A:ILE:HG23  | 1:85:A:TYR:H     | 5                   | 0.29     | 0.08                | 0.31       |
| (1,1470) | 1:86:A:ILE:HG22  | 1:85:A:TYR:H     | 5                   | 0.29     | 0.08                | 0.31       |
| (1,764)  | 1:44:A:GLU:HG2   | 1:128:A:ASN:HD21 | 5                   | 0.25     | 0.04                | 0.26       |
| (1,12)   | 1:105:A:ARG:HD2  | 1:105:A:ARG:HA   | 5                   | 0.23     | 0.04                | 0.23       |
| (1,12)   | 1:105:A:ARG:HD3  | 1:105:A:ARG:HA   | 5                   | 0.23     | 0.04                | 0.23       |
| (1,880)  | 1:29:A:GLU:H     | 1:29:A:GLU:HG3   | 5                   | 0.21     | 0.05                | 0.23       |
| (1,553)  | 1:85:A:TYR:HB3   | 1:85:A:TYR:H     | 5                   | 0.2      | 0.04                | 0.19       |
| (1,1345) | 1:126:A:ILE:H    | 1:113:A:SER:HB2  | 5                   | 0.19     | 0.04                | 0.18       |
| (1,514)  | 1:51:A:LYS:HG3   | 1:56:A:ARG:HA    | 5                   | 0.18     | 0.03                | 0.18       |
| (1,1380) | 1:132:A:GLY:HA2  | 1:40:A:ILE:H     | 5                   | 0.16     | 0.05                | 0.14       |
| (1,1380) | 1:132:A:GLY:HA3  | 1:40:A:ILE:H     | 5                   | 0.16     | 0.05                | 0.14       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,128)  | 1:41:A:VAL:HA   | 1:44:A:GLU:HB3   | 5                   | 0.15     | 0.03                | 0.15       |
| (1,534)  | 1:109:A:VAL:HB  | 1:57:A:TYR:HD1   | 5                   | 0.14     | 0.03                | 0.14       |
| (1,534)  | 1:109:A:VAL:HB  | 1:57:A:TYR:HD2   | 5                   | 0.14     | 0.03                | 0.14       |
| (1,1508) | 1:66:A:ALA:HA   | 1:69:A:LYS:H     | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1053) | 1:53:A:ASP:HB3  | 1:54:A:ASN:H     | 5                   | 0.14     | 0.02                | 0.15       |
| (1,1507) | 1:58:A:PRO:HB2  | 1:100:A:LEU:HD21 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1507) | 1:58:A:PRO:HB2  | 1:100:A:LEU:HD23 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1507) | 1:58:A:PRO:HB2  | 1:100:A:LEU:HD22 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1087) | 1:113:A:SER:H   | 1:112:A:PHE:HB3  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,106)  | 1:40:A:ILE:HA   | 1:40:A:ILE:HD11  | 5                   | 0.12     | 0.01                | 0.11       |
| (1,106)  | 1:40:A:ILE:HA   | 1:40:A:ILE:HD12  | 5                   | 0.12     | 0.01                | 0.11       |
| (1,106)  | 1:40:A:ILE:HA   | 1:40:A:ILE:HD13  | 5                   | 0.12     | 0.01                | 0.11       |
| (1,1282) | 1:98:A:TYR:H    | 1:99:A:GLN:HE21  | 4                   | 0.98     | 0.57                | 1.02       |
| (1,633)  | 1:79:A:SER:HB3  | 1:79:A:SER:H     | 4                   | 0.4      | 0.03                | 0.41       |
| (1,304)  | 1:72:A:THR:HG23 | 1:73:A:THR:H     | 4                   | 0.39     | 0.04                | 0.4        |
| (1,304)  | 1:72:A:THR:HG21 | 1:73:A:THR:H     | 4                   | 0.39     | 0.04                | 0.4        |
| (1,304)  | 1:72:A:THR:HG22 | 1:73:A:THR:H     | 4                   | 0.39     | 0.04                | 0.4        |
| (1,1028) | 1:86:A:ILE:H    | 1:46:A:ALA:HB3   | 4                   | 0.3      | 0.03                | 0.31       |
| (1,1028) | 1:86:A:ILE:H    | 1:46:A:ALA:HB2   | 4                   | 0.3      | 0.03                | 0.31       |
| (1,1028) | 1:86:A:ILE:H    | 1:46:A:ALA:HB1   | 4                   | 0.3      | 0.03                | 0.31       |
| (1,207)  | 1:122:A:THR:HB  | 1:123:A:ASP:HB2  | 4                   | 0.18     | 0.08                | 0.14       |
| (1,207)  | 1:122:A:THR:HB  | 1:123:A:ASP:HB3  | 4                   | 0.18     | 0.08                | 0.14       |
| (1,1484) | 1:64:A:LEU:HD22 | 1:63:A:GLY:HA2   | 4                   | 0.18     | 0.04                | 0.18       |
| (1,1484) | 1:64:A:LEU:HD21 | 1:63:A:GLY:HA2   | 4                   | 0.18     | 0.04                | 0.18       |
| (1,1595) | 1:32:A:ASP:H    | 1:30:A:LYS:HB3   | 4                   | 0.17     | 0.04                | 0.18       |
| (1,1175) | 1:26:A:GLY:H    | 1:28:A:LYS:HA    | 4                   | 0.17     | 0.02                | 0.16       |
| (1,133)  | 1:41:A:VAL:HG22 | 1:41:A:VAL:H     | 4                   | 0.13     | 0.02                | 0.14       |
| (1,133)  | 1:41:A:VAL:HG21 | 1:41:A:VAL:H     | 4                   | 0.13     | 0.02                | 0.14       |
| (1,133)  | 1:41:A:VAL:HG23 | 1:41:A:VAL:H     | 4                   | 0.13     | 0.02                | 0.14       |
| (1,721)  | 1:30:A:LYS:HA   | 1:32:A:ASP:H     | 4                   | 0.12     | 0.01                | 0.12       |
| (1,704)  | 1:104:A:GLY:HA3 | 1:106:A:HIS:H    | 4                   | 0.12     | 0.02                | 0.11       |
| (1,1515) | 1:28:A:LYS:HB3  | 1:28:A:LYS:HE3   | 3                   | 0.75     | 0.1                 | 0.81       |
| (1,1515) | 1:30:A:LYS:HB3  | 1:30:A:LYS:HE3   | 3                   | 0.75     | 0.1                 | 0.81       |
| (1,1515) | 1:30:A:LYS:HB3  | 1:30:A:LYS:HE2   | 3                   | 0.75     | 0.1                 | 0.81       |
| (1,1473) | 1:78:A:ARG:HD2  | 1:78:A:ARG:H     | 3                   | 0.44     | 0.08                | 0.47       |
| (1,1472) | 1:78:A:ARG:HD3  | 1:78:A:ARG:HB2   | 3                   | 0.32     | 0.05                | 0.33       |
| (1,745)  | 1:140:A:SER:HB3 | 1:138:A:ASN:HD22 | 3                   | 0.31     | 0.15                | 0.24       |
| (1,772)  | 1:105:A:ARG:HG2 | 1:106:A:HIS:HD2  | 3                   | 0.31     | 0.01                | 0.31       |
| (1,421)  | 1:129:A:TRP:HB2 | 1:106:A:HIS:HB2  | 3                   | 0.29     | 0.15                | 0.31       |
| (1,275)  | 1:119:A:MET:HB3 | 1:122:A:THR:HG21 | 3                   | 0.29     | 0.16                | 0.24       |
| (1,275)  | 1:119:A:MET:HB3 | 1:122:A:THR:HG23 | 3                   | 0.29     | 0.16                | 0.24       |
| (1,275)  | 1:119:A:MET:HB3 | 1:122:A:THR:HG22 | 3                   | 0.29     | 0.16                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1439) | 1:79:A:SER:H     | 1:78:A:ARG:HD3   | 3                   | 0.27     | 0.08                | 0.27       |
| (1,763)  | 1:44:A:GLU:HG2   | 1:45:A:SER:H     | 3                   | 0.26     | 0.03                | 0.26       |
| (1,1006) | 1:108:A:LYS:HB2  | 1:109:A:VAL:H    | 3                   | 0.26     | 0.13                | 0.23       |
| (1,469)  | 1:44:A:GLU:HG3   | 1:44:A:GLU:HA    | 3                   | 0.24     | 0.02                | 0.24       |
| (1,1007) | 1:109:A:VAL:H    | 1:108:A:LYS:HD3  | 3                   | 0.23     | 0.05                | 0.21       |
| (1,1007) | 1:109:A:VAL:H    | 1:108:A:LYS:HD2  | 3                   | 0.23     | 0.05                | 0.21       |
| (1,1587) | 1:127:A:GLY:H    | 1:40:A:ILE:HD13  | 3                   | 0.23     | 0.02                | 0.22       |
| (1,1587) | 1:127:A:GLY:H    | 1:40:A:ILE:HD12  | 3                   | 0.23     | 0.02                | 0.22       |
| (1,1587) | 1:127:A:GLY:H    | 1:40:A:ILE:HG22  | 3                   | 0.23     | 0.02                | 0.22       |
| (1,143)  | 1:133:A:THR:HB   | 1:134:A:SER:H    | 3                   | 0.21     | 0.04                | 0.24       |
| (1,29)   | 1:105:A:ARG:HA   | 1:105:A:ARG:HB3  | 3                   | 0.21     | 0.02                | 0.21       |
| (1,278)  | 1:86:A:ILE:HD13  | 1:67:A:LEU:HB3   | 3                   | 0.2      | 0.02                | 0.22       |
| (1,278)  | 1:86:A:ILE:HD11  | 1:67:A:LEU:HB3   | 3                   | 0.2      | 0.02                | 0.22       |
| (1,1576) | 1:83:A:ASP:H     | 1:84:A:GLY:HA3   | 3                   | 0.19     | 0.09                | 0.14       |
| (1,1301) | 1:85:A:TYR:H     | 1:85:A:TYR:HE1   | 3                   | 0.19     | 0.01                | 0.18       |
| (1,1301) | 1:85:A:TYR:H     | 1:85:A:TYR:HE2   | 3                   | 0.19     | 0.01                | 0.18       |
| (1,163)  | 1:88:A:ARG:HB3   | 1:88:A:ARG:H     | 3                   | 0.16     | 0.02                | 0.15       |
| (1,1502) | 1:57:A:TYR:HA    | 1:57:A:TYR:HD1   | 3                   | 0.15     | 0.02                | 0.15       |
| (1,1502) | 1:57:A:TYR:HA    | 1:57:A:TYR:HD2   | 3                   | 0.15     | 0.02                | 0.15       |
| (1,1570) | 1:79:A:SER:H     | 1:53:A:ASP:HB3   | 3                   | 0.15     | 0.04                | 0.12       |
| (1,783)  | 1:125:A:ASP:HA   | 1:126:A:ILE:HB   | 3                   | 0.14     | 0.03                | 0.13       |
| (1,906)  | 1:107:A:GLY:H    | 1:105:A:ARG:H    | 3                   | 0.14     | 0.02                | 0.14       |
| (1,1497) | 1:73:A:THR:HB    | 1:62:A:GLN:HG2   | 3                   | 0.13     | 0.03                | 0.11       |
| (1,30)   | 1:78:A:ARG:HA    | 1:78:A:ARG:HB3   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,30)   | 1:78:A:ARG:HA    | 1:78:A:ARG:HB2   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,896)  | 1:53:A:ASP:HB3   | 1:53:A:ASP:H     | 3                   | 0.12     | 0.01                | 0.12       |
| (1,332)  | 1:112:A:PHE:HB2  | 1:129:A:TRP:HZ3  | 3                   | 0.12     | 0.01                | 0.13       |
| (1,879)  | 1:48:A:ASP:H     | 1:44:A:GLU:HA    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1540) | 1:57:A:TYR:H     | 1:56:A:ARG:H     | 3                   | 0.11     | 0.01                | 0.1        |
| (1,1528) | 1:31:A:ALA:HB3   | 1:27:A:ASN:HB3   | 2                   | 0.74     | 0.42                | 0.74       |
| (1,1528) | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB2   | 2                   | 0.74     | 0.42                | 0.74       |
| (1,338)  | 1:52:A:LEU:HD22  | 1:52:A:LEU:H     | 2                   | 0.68     | 0.02                | 0.68       |
| (1,395)  | 1:97:A:GLU:HB2   | 1:97:A:GLU:H     | 2                   | 0.64     | 0.0                 | 0.64       |
| (1,1353) | 1:138:A:ASN:HD21 | 1:138:A:ASN:HA   | 2                   | 0.56     | 0.32                | 0.56       |
| (1,183)  | 1:32:A:ASP:HB3   | 1:28:A:LYS:HG3   | 2                   | 0.54     | 0.18                | 0.54       |
| (1,1349) | 1:52:A:LEU:H     | 1:48:A:ASP:HB3   | 2                   | 0.49     | 0.39                | 0.49       |
| (1,286)  | 1:132:A:GLY:HA2  | 1:133:A:THR:HG21 | 2                   | 0.4      | 0.07                | 0.4        |
| (1,286)  | 1:132:A:GLY:HA3  | 1:133:A:THR:HG22 | 2                   | 0.4      | 0.07                | 0.4        |
| (1,220)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HD2  | 2                   | 0.33     | 0.05                | 0.33       |
| (1,650)  | 1:32:A:ASP:HB2   | 1:93:A:PRO:HB2   | 2                   | 0.31     | 0.07                | 0.31       |
| (1,1590) | 1:55:A:SER:H     | 1:51:A:LYS:HB2   | 2                   | 0.29     | 0.01                | 0.29       |
| (1,83)   | 1:36:A:ALA:HB3   | 1:94:A:TRP:HH2   | 2                   | 0.27     | 0.01                | 0.27       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,83)   | 1:36:A:ALA:HB1   | 1:94:A:TRP:HH2   | 2                   | 0.27     | 0.01                | 0.27       |
| (1,848)  | 1:70:A:LYS:H     | 1:70:A:LYS:HG2   | 2                   | 0.26     | 0.02                | 0.26       |
| (1,848)  | 1:70:A:LYS:H     | 1:70:A:LYS:HG3   | 2                   | 0.26     | 0.02                | 0.26       |
| (1,1269) | 1:55:A:SER:H     | 1:51:A:LYS:HD3   | 2                   | 0.24     | 0.05                | 0.24       |
| (1,407)  | 1:61:A:GLU:HA    | 1:61:A:GLU:HG3   | 2                   | 0.23     | 0.03                | 0.23       |
| (1,888)  | 1:108:A:LYS:HB3  | 1:108:A:LYS:H    | 2                   | 0.23     | 0.04                | 0.23       |
| (1,1339) | 1:40:A:ILE:HG22  | 1:128:A:ASN:HD22 | 2                   | 0.2      | 0.02                | 0.2        |
| (1,1339) | 1:40:A:ILE:HG23  | 1:128:A:ASN:HD22 | 2                   | 0.2      | 0.02                | 0.2        |
| (1,434)  | 1:41:A:VAL:HG11  | 1:38:A:SER:H     | 2                   | 0.18     | 0.06                | 0.18       |
| (1,674)  | 1:109:A:VAL:HG21 | 1:57:A:TYR:HD2   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,674)  | 1:109:A:VAL:HG23 | 1:57:A:TYR:HD2   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,420)  | 1:48:A:ASP:HA    | 1:57:A:TYR:HE1   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,420)  | 1:48:A:ASP:HA    | 1:57:A:TYR:HE2   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,242)  | 1:54:A:ASN:HB2   | 1:77:A:PRO:HA    | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1459) | 1:86:A:ILE:HB    | 1:86:A:ILE:HG21  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1459) | 1:86:A:ILE:HB    | 1:86:A:ILE:HG22  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,156)  | 1:80:A:TYR:HB2   | 1:85:A:TYR:HD2   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,464)  | 1:82:A:GLN:HG3   | 1:82:A:GLN:HA    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1283) | 1:73:A:THR:H     | 1:62:A:GLN:HB3   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1454) | 1:40:A:ILE:HB    | 1:111:A:VAL:HG23 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,186)  | 1:46:A:ALA:HA    | 1:46:A:ALA:HB1   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,186)  | 1:46:A:ALA:HA    | 1:46:A:ALA:HB3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,902)  | 1:107:A:GLY:H    | 1:104:A:GLY:HA3  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,817)  | 1:56:A:ARG:H     | 1:56:A:ARG:HD3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1348) | 1:126:A:ILE:H    | 1:112:A:PHE:HD1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1348) | 1:126:A:ILE:H    | 1:112:A:PHE:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |

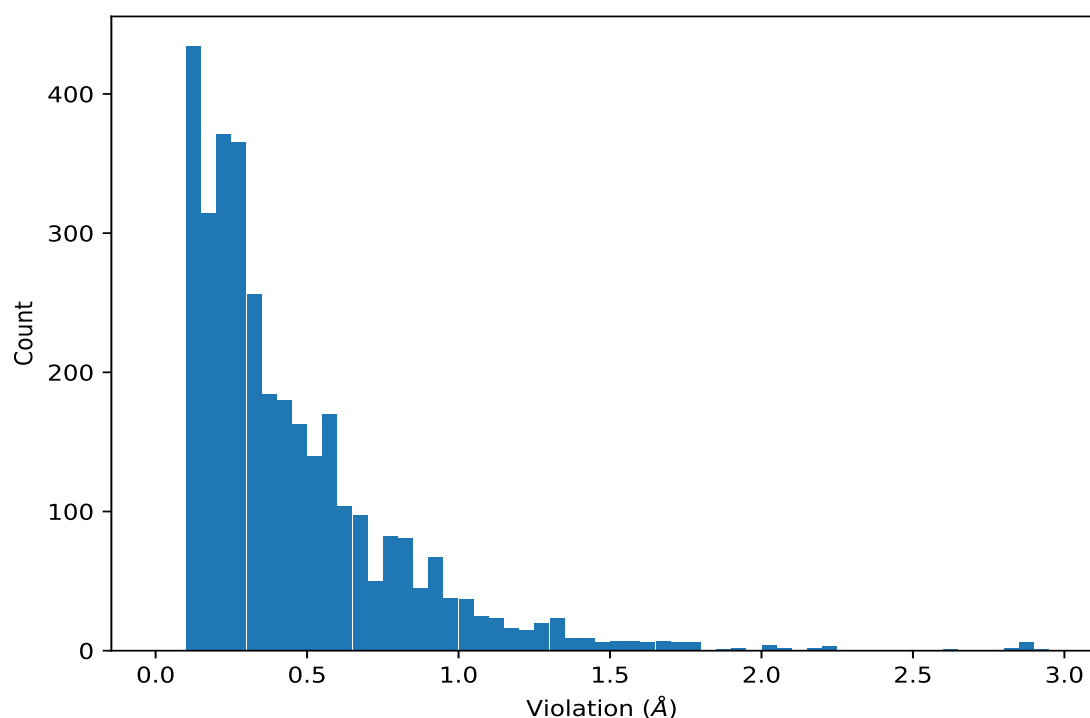
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

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

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

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





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

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

| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 3        | 2.92          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 5        | 2.9           |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 4        | 2.89          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 9        | 2.89          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 8        | 2.86          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 2        | 2.85          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 6        | 2.85          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 7        | 2.83          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 10       | 2.82          |
| (1,1357) | 1:62:A:GLN:HE21 | 1:63:A:GLY:HA3  | 1        | 2.63          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 4        | 2.23          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 8        | 2.23          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 6        | 2.21          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 2        | 2.19          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 3        | 2.17          |
| (1,787)  | 1:96:A:ALA:HB2  | 1:114:A:TYR:HB3 | 7        | 2.08          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 7        | 2.06          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 1        | 2.04          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 9        | 2.02          |
| (1,632)  | 1:79:A:SER:HB3  | 1:78:A:ARG:HG3  | 2        | 2.01          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 10       | 2.01          |
| (1,632)  | 1:79:A:SER:HB3  | 1:78:A:ARG:HG3  | 7        | 1.94          |
| (1,341)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB2  | 5        | 1.93          |
| (1,1186) | 1:62:A:GLN:HE22 | 1:75:A:PRO:HB2  | 1        | 1.86          |
| (1,541)  | 1:85:A:TYR:HE2  | 1:84:A:GLY:HA3  | 3        | 1.79          |
| (1,768)  | 1:67:A:LEU:HB2  | 1:85:A:TYR:HB3  | 3        | 1.78          |
| (1,768)  | 1:67:A:LEU:HB2  | 1:85:A:TYR:HB3  | 8        | 1.76          |
| (1,801)  | 1:79:A:SER:HB3  | 1:78:A:ARG:HB2  | 5        | 1.75          |
| (1,630)  | 1:32:A:ASP:HB3  | 1:31:A:ALA:HB2  | 3        | 1.75          |
| (1,541)  | 1:85:A:TYR:HE2  | 1:84:A:GLY:HA3  | 10       | 1.75          |
| (1,541)  | 1:85:A:TYR:HE1  | 1:84:A:GLY:HA3  | 5        | 1.73          |
| (1,1186) | 1:62:A:GLN:HE22 | 1:75:A:PRO:HB2  | 10       | 1.72          |
| (1,768)  | 1:67:A:LEU:HB2  | 1:85:A:TYR:HB3  | 4        | 1.72          |
| (1,719)  | 1:45:A:SER:HB2  | 1:48:A:ASP:HB2  | 5        | 1.72          |
| (1,541)  | 1:85:A:TYR:HE1  | 1:84:A:GLY:HA3  | 8        | 1.72          |
| (1,541)  | 1:85:A:TYR:HE2  | 1:84:A:GLY:HA3  | 4        | 1.71          |
| (1,1317) | 1:97:A:GLU:HA   | 1:91:A:GLN:HE21 | 10       | 1.7           |
| (1,768)  | 1:67:A:LEU:HB2  | 1:85:A:TYR:HB3  | 2        | 1.7           |
| (1,630)  | 1:32:A:ASP:HB3  | 1:31:A:ALA:HB2  | 2        | 1.69          |
| (1,51)   | 1:33:A:ARG:HB3  | 1:116:A:PRO:HG2 | 8        | 1.69          |
| (1,541)  | 1:85:A:TYR:HE2  | 1:84:A:GLY:HA3  | 2        | 1.68          |
| (1,966)  | 1:96:A:ALA:H    | 1:94:A:TRP:HZ3  | 4        | 1.67          |
| (1,51)   | 1:33:A:ARG:HB3  | 1:116:A:PRO:HG2 | 3        | 1.66          |
| (1,1525) | 1:75:A:PRO:HG3  | 1:50:A:TYR:HE1  | 3        | 1.63          |
| (1,51)   | 1:33:A:ARG:HB3  | 1:116:A:PRO:HG2 | 6        | 1.63          |
| (1,768)  | 1:67:A:LEU:HB2  | 1:85:A:TYR:HB3  | 9        | 1.62          |
| (1,541)  | 1:85:A:TYR:HE1  | 1:84:A:GLY:HA3  | 6        | 1.62          |
| (1,51)   | 1:33:A:ARG:HB3  | 1:116:A:PRO:HG2 | 7        | 1.61          |
| (1,634)  | 1:79:A:SER:HB3  | 1:54:A:ASN:HA   | 7        | 1.6           |
| (1,768)  | 1:67:A:LEU:HB2  | 1:85:A:TYR:HB3  | 10       | 1.59          |
| (1,1417) | 1:33:A:ARG:H    | 1:116:A:PRO:HG2 | 6        | 1.58          |
| (1,1186) | 1:62:A:GLN:HE22 | 1:75:A:PRO:HB2  | 4        | 1.58          |
| (1,541)  | 1:85:A:TYR:HE2  | 1:84:A:GLY:HA3  | 7        | 1.57          |
| (1,541)  | 1:85:A:TYR:HE1  | 1:84:A:GLY:HA3  | 1        | 1.56          |
| (1,336)  | 1:52:A:LEU:HD21 | 1:48:A:ASP:HB3  | 5        | 1.56          |
| (1,1186) | 1:62:A:GLN:HE22 | 1:75:A:PRO:HB2  | 6        | 1.55          |
| (1,1282) | 1:98:A:TYR:H    | 1:99:A:GLN:HE21 | 7        | 1.54          |
| (1,1282) | 1:98:A:TYR:H    | 1:99:A:GLN:HE21 | 10       | 1.54          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2  | 2        | 1.54          |
| (1,51)   | 1:33:A:ARG:HB3   | 1:116:A:PRO:HG2 | 2        | 1.53          |
| (1,1186) | 1:62:A:GLN:HE22  | 1:75:A:PRO:HB2  | 3        | 1.52          |
| (1,51)   | 1:33:A:ARG:HB3   | 1:116:A:PRO:HG2 | 5        | 1.5           |
| (1,51)   | 1:33:A:ARG:HB3   | 1:116:A:PRO:HG2 | 9        | 1.5           |
| (1,1186) | 1:62:A:GLN:HE22  | 1:75:A:PRO:HB2  | 7        | 1.49          |
| (1,787)  | 1:96:A:ALA:HB1   | 1:114:A:TYR:HB3 | 10       | 1.49          |
| (1,768)  | 1:67:A:LEU:HB2   | 1:85:A:TYR:HB3  | 5        | 1.48          |
| (1,634)  | 1:79:A:SER:HB3   | 1:54:A:ASN:HA   | 5        | 1.48          |
| (1,966)  | 1:96:A:ALA:H     | 1:94:A:TRP:HZ3  | 10       | 1.47          |
| (1,634)  | 1:79:A:SER:HB3   | 1:54:A:ASN:HA   | 2        | 1.46          |
| (1,1186) | 1:62:A:GLN:HE22  | 1:75:A:PRO:HB2  | 2        | 1.45          |
| (1,1317) | 1:97:A:GLU:HA    | 1:91:A:GLN:HE21 | 4        | 1.44          |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB3  | 9        | 1.44          |
| (1,768)  | 1:67:A:LEU:HB2   | 1:85:A:TYR:HB3  | 6        | 1.43          |
| (1,1186) | 1:62:A:GLN:HE22  | 1:75:A:PRO:HB2  | 5        | 1.42          |
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2  | 7        | 1.42          |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA  | 8        | 1.42          |
| (1,1520) | 1:111:A:VAL:HG13 | 1:110:A:ASP:HB2 | 3        | 1.41          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2 | 8        | 1.41          |
| (1,1520) | 1:111:A:VAL:HG12 | 1:110:A:ASP:HB2 | 10       | 1.39          |
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2  | 3        | 1.39          |
| (1,768)  | 1:67:A:LEU:HB2   | 1:85:A:TYR:HB3  | 1        | 1.38          |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG   | 8        | 1.37          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3 | 2        | 1.36          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3 | 8        | 1.36          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE1  | 1        | 1.35          |
| (1,1522) | 1:105:A:ARG:HD2  | 1:102:A:SER:HA  | 8        | 1.35          |
| (1,768)  | 1:67:A:LEU:HB2   | 1:85:A:TYR:HB3  | 7        | 1.35          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE2  | 6        | 1.34          |
| (1,787)  | 1:96:A:ALA:HB1   | 1:114:A:TYR:HB3 | 1        | 1.34          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD23 | 7        | 1.34          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD23 | 10       | 1.34          |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG   | 10       | 1.34          |
| (1,51)   | 1:33:A:ARG:HB3   | 1:116:A:PRO:HG2 | 1        | 1.34          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2 | 5        | 1.33          |
| (1,1317) | 1:97:A:GLU:HA    | 1:91:A:GLN:HE21 | 8        | 1.33          |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA  | 1        | 1.33          |
| (1,541)  | 1:85:A:TYR:HE1   | 1:84:A:GLY:HA3  | 9        | 1.32          |
| (1,51)   | 1:33:A:ARG:HB3   | 1:116:A:PRO:HG2 | 4        | 1.32          |
| (1,492)  | 1:122:A:THR:HG22 | 1:119:A:MET:HG2 | 10       | 1.31          |
| (1,51)   | 1:33:A:ARG:HB3   | 1:116:A:PRO:HG2 | 10       | 1.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD12  | 10       | 1.3           |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 7        | 1.3           |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 9        | 1.3           |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 2        | 1.3           |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 7        | 1.3           |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 2        | 1.3           |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 3        | 1.3           |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 4        | 1.3           |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 6        | 1.3           |
| (1,492)  | 1:122:A:THR:HG22 | 1:119:A:MET:HG2  | 6        | 1.3           |
| (1,1505) | 1:66:A:ALA:HB1   | 1:63:A:GLY:HA3   | 3        | 1.29          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 6        | 1.29          |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 4        | 1.29          |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 6        | 1.29          |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 9        | 1.29          |
| (1,1522) | 1:105:A:ARG:HD2  | 1:102:A:SER:HA   | 1        | 1.28          |
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD22  | 9        | 1.28          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2  | 9        | 1.28          |
| (1,1317) | 1:97:A:GLU:HA    | 1:91:A:GLN:HE21  | 7        | 1.28          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 5        | 1.28          |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 5        | 1.28          |
| (1,1505) | 1:66:A:ALA:HB2   | 1:63:A:GLY:HA3   | 6        | 1.27          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 3        | 1.27          |
| (1,1520) | 1:111:A:VAL:HG12 | 1:110:A:ASP:HB2  | 7        | 1.26          |
| (1,1520) | 1:111:A:VAL:HG12 | 1:128:A:ASN:HB2  | 8        | 1.26          |
| (1,1505) | 1:66:A:ALA:HB2   | 1:64:A:LEU:HA    | 2        | 1.26          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 3        | 1.26          |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 7        | 1.26          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 6        | 1.25          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 10       | 1.25          |
| (1,1505) | 1:66:A:ALA:HB2   | 1:64:A:LEU:HA    | 7        | 1.24          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 1        | 1.24          |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 9        | 1.24          |
| (1,1520) | 1:111:A:VAL:HG12 | 1:128:A:ASN:HB2  | 9        | 1.23          |
| (1,1505) | 1:66:A:ALA:HB3   | 1:63:A:GLY:HA3   | 1        | 1.23          |
| (1,1505) | 1:66:A:ALA:HB1   | 1:64:A:LEU:HA    | 8        | 1.23          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 4        | 1.23          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 10       | 1.23          |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 5        | 1.23          |
| (1,229)  | 1:63:A:GLY:HA2   | 1:111:A:VAL:HG12 | 1        | 1.23          |
| (1,1520) | 1:111:A:VAL:HG11 | 1:110:A:ASP:HB2  | 1        | 1.21          |
| (1,1520) | 1:111:A:VAL:HG12 | 1:110:A:ASP:HB2  | 2        | 1.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1520) | 1:111:A:VAL:HG12 | 1:128:A:ASN:HB2  | 4        | 1.21          |
| (1,1520) | 1:111:A:VAL:HG12 | 1:110:A:ASP:HB2  | 6        | 1.21          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2  | 3        | 1.21          |
| (1,1505) | 1:66:A:ALA:HB2   | 1:63:A:GLY:HA3   | 4        | 1.2           |
| (1,1505) | 1:66:A:ALA:HB1   | 1:63:A:GLY:HA3   | 9        | 1.2           |
| (1,1505) | 1:66:A:ALA:HB2   | 1:63:A:GLY:HA3   | 10       | 1.2           |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 3        | 1.2           |
| (1,432)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:HB2   | 1        | 1.2           |
| (1,1520) | 1:111:A:VAL:HG12 | 1:128:A:ASN:HB2  | 5        | 1.19          |
| (1,589)  | 1:130:A:ASN:HB3  | 1:131:A:VAL:HA   | 10       | 1.19          |
| (1,1505) | 1:66:A:ALA:HB3   | 1:63:A:GLY:HA3   | 5        | 1.18          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2  | 7        | 1.18          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 8        | 1.18          |
| (1,787)  | 1:96:A:ALA:HB3   | 1:114:A:TYR:HB3  | 9        | 1.18          |
| (1,432)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:HB1   | 9        | 1.18          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 1        | 1.17          |
| (1,1528) | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB2   | 3        | 1.16          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2  | 4        | 1.16          |
| (1,492)  | 1:122:A:THR:HG23 | 1:119:A:MET:HG2  | 2        | 1.16          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2  | 2        | 1.15          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 7        | 1.15          |
| (1,432)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:HB1   | 3        | 1.15          |
| (1,432)  | 1:41:A:VAL:HG13  | 1:42:A:ALA:HB1   | 4        | 1.15          |
| (1,1522) | 1:105:A:ARG:HD2  | 1:102:A:SER:HA   | 6        | 1.14          |
| (1,1317) | 1:97:A:GLU:HA    | 1:91:A:GLN:HE21  | 6        | 1.14          |
| (1,1186) | 1:62:A:GLN:HE22  | 1:75:A:PRO:HB2   | 9        | 1.14          |
| (1,492)  | 1:122:A:THR:HG23 | 1:119:A:MET:HG2  | 8        | 1.14          |
| (1,432)  | 1:41:A:VAL:HG13  | 1:42:A:ALA:HB3   | 7        | 1.14          |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG3   | 8        | 1.14          |
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD11  | 1        | 1.13          |
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2   | 1        | 1.13          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 4        | 1.13          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 5        | 1.13          |
| (1,787)  | 1:96:A:ALA:HB3   | 1:114:A:TYR:HB3  | 3        | 1.13          |
| (1,432)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:HB3   | 8        | 1.13          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 9        | 1.12          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 4        | 1.11          |
| (1,492)  | 1:122:A:THR:HG21 | 1:119:A:MET:HG2  | 1        | 1.11          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE2   | 5        | 1.1           |
| (1,634)  | 1:79:A:SER:HB3   | 1:54:A:ASN:HA    | 3        | 1.1           |
| (1,229)  | 1:63:A:GLY:HA2   | 1:111:A:VAL:HG11 | 3        | 1.1           |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 2        | 1.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 3        | 1.09          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 4        | 1.09          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 3        | 1.09          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 9        | 1.09          |
| (1,794)  | 1:106:A:HIS:HB3  | 1:105:A:ARG:H    | 2        | 1.09          |
| (1,773)  | 1:63:A:GLY:HA3   | 1:47:A:LEU:HG    | 1        | 1.09          |
| (1,492)  | 1:122:A:THR:HG21 | 1:119:A:MET:HG2  | 4        | 1.09          |
| (1,432)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:HB3   | 6        | 1.09          |
| (1,432)  | 1:41:A:VAL:HG12  | 1:42:A:ALA:HB1   | 10       | 1.09          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 7        | 1.08          |
| (1,898)  | 1:52:A:LEU:HD12  | 1:53:A:ASP:H     | 10       | 1.08          |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB3   | 8        | 1.08          |
| (1,1535) | 1:62:A:GLN:H     | 1:66:A:ALA:HB3   | 2        | 1.07          |
| (1,432)  | 1:41:A:VAL:HG13  | 1:42:A:ALA:HB3   | 2        | 1.07          |
| (1,1535) | 1:62:A:GLN:H     | 1:66:A:ALA:HB3   | 10       | 1.06          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE1   | 10       | 1.06          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 5        | 1.06          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 9        | 1.06          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 7        | 1.06          |
| (1,787)  | 1:96:A:ALA:HB1   | 1:114:A:TYR:HB3  | 8        | 1.06          |
| (1,432)  | 1:41:A:VAL:HG13  | 1:42:A:ALA:HB1   | 5        | 1.06          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 6        | 1.05          |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 8        | 1.05          |
| (1,898)  | 1:52:A:LEU:HD12  | 1:53:A:ASP:H     | 7        | 1.05          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB3  | 6        | 1.05          |
| (1,1535) | 1:62:A:GLN:H     | 1:66:A:ALA:HB1   | 1        | 1.04          |
| (1,1535) | 1:62:A:GLN:H     | 1:60:A:THR:HG23  | 3        | 1.04          |
| (1,1535) | 1:62:A:GLN:H     | 1:66:A:ALA:HB3   | 7        | 1.04          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 2        | 1.04          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG22  | 10       | 1.04          |
| (1,492)  | 1:122:A:THR:HG23 | 1:119:A:MET:HG2  | 3        | 1.04          |
| (1,492)  | 1:122:A:THR:HG21 | 1:119:A:MET:HG2  | 7        | 1.04          |
| (1,229)  | 1:63:A:GLY:HA2   | 1:111:A:VAL:HG13 | 2        | 1.04          |
| (1,229)  | 1:63:A:GLY:HA2   | 1:111:A:VAL:HG13 | 9        | 1.04          |
| (1,1317) | 1:97:A:GLU:HA    | 1:91:A:GLN:HE21  | 3        | 1.03          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 1        | 1.03          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 8        | 1.03          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 5        | 1.03          |
| (1,1212) | 1:62:A:GLN:H     | 1:62:A:GLN:HE21  | 3        | 1.03          |
| (1,1535) | 1:62:A:GLN:H     | 1:66:A:ALA:HB2   | 9        | 1.02          |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2  | 1        | 1.02          |
| (1,1307) | 1:110:A:ASP:H    | 1:100:A:LEU:HB3  | 2        | 1.02          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1307) | 1:110:A:ASP:H   | 1:100:A:LEU:HB3  | 10       | 1.02          |
| (1,1303) | 1:125:A:ASP:H   | 1:122:A:THR:HG22 | 1        | 1.02          |
| (1,1303) | 1:125:A:ASP:H   | 1:122:A:THR:HG23 | 5        | 1.02          |
| (1,912)  | 1:117:A:ASP:H   | 1:116:A:PRO:HG3  | 2        | 1.02          |
| (1,744)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB3   | 7        | 1.02          |
| (1,229)  | 1:63:A:GLY:HA2  | 1:111:A:VAL:HG13 | 7        | 1.02          |
| (1,1527) | 1:66:A:ALA:HB1  | 1:68:A:VAL:H     | 3        | 1.01          |
| (1,1522) | 1:105:A:ARG:HD2 | 1:102:A:SER:HA   | 7        | 1.01          |
| (1,1250) | 1:94:A:TRP:HE1  | 1:116:A:PRO:HG2  | 10       | 1.01          |
| (1,1212) | 1:62:A:GLN:H    | 1:62:A:GLN:HE21  | 9        | 1.01          |
| (1,1172) | 1:101:A:VAL:H   | 1:109:A:VAL:HG11 | 9        | 1.01          |
| (1,801)  | 1:79:A:SER:HB3  | 1:78:A:ARG:HB2   | 10       | 1.01          |
| (1,1554) | 1:66:A:ALA:H    | 1:58:A:PRO:HB3   | 2        | 1.0           |
| (1,1554) | 1:66:A:ALA:H    | 1:64:A:LEU:HB2   | 3        | 1.0           |
| (1,1535) | 1:62:A:GLN:H    | 1:66:A:ALA:HB3   | 6        | 1.0           |
| (1,1250) | 1:94:A:TRP:HE1  | 1:116:A:PRO:HG2  | 8        | 1.0           |
| (1,1212) | 1:62:A:GLN:H    | 1:62:A:GLN:HE21  | 1        | 1.0           |
| (1,1212) | 1:62:A:GLN:H    | 1:62:A:GLN:HE21  | 7        | 1.0           |
| (1,898)  | 1:52:A:LEU:HD22 | 1:53:A:ASP:H     | 6        | 1.0           |
| (1,229)  | 1:63:A:GLY:HA2  | 1:111:A:VAL:HG13 | 10       | 1.0           |
| (1,1527) | 1:66:A:ALA:HB2  | 1:68:A:VAL:H     | 10       | 0.99          |
| (1,1303) | 1:125:A:ASP:H   | 1:122:A:THR:HG21 | 9        | 0.99          |
| (1,1172) | 1:101:A:VAL:H   | 1:109:A:VAL:HG13 | 3        | 0.99          |
| (1,736)  | 1:86:A:ILE:HG21 | 1:85:A:TYR:HD1   | 6        | 0.99          |
| (1,229)  | 1:63:A:GLY:HA2  | 1:111:A:VAL:HG13 | 5        | 0.99          |
| (1,229)  | 1:63:A:GLY:HA2  | 1:111:A:VAL:HG13 | 6        | 0.99          |
| (1,154)  | 1:80:A:TYR:HB2  | 1:77:A:PRO:HB2   | 7        | 0.99          |
| (1,1554) | 1:66:A:ALA:H    | 1:64:A:LEU:HB3   | 6        | 0.98          |
| (1,1303) | 1:125:A:ASP:H   | 1:122:A:THR:HG23 | 10       | 0.98          |
| (1,1212) | 1:62:A:GLN:H    | 1:62:A:GLN:HE21  | 2        | 0.98          |
| (1,1212) | 1:62:A:GLN:H    | 1:62:A:GLN:HE21  | 4        | 0.98          |
| (1,1212) | 1:62:A:GLN:H    | 1:62:A:GLN:HE21  | 5        | 0.98          |
| (1,744)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB3   | 1        | 0.98          |
| (1,736)  | 1:86:A:ILE:HG23 | 1:85:A:TYR:HD2   | 4        | 0.98          |
| (1,1554) | 1:66:A:ALA:H    | 1:64:A:LEU:HB2   | 1        | 0.97          |
| (1,1554) | 1:66:A:ALA:H    | 1:64:A:LEU:HB2   | 8        | 0.97          |
| (1,1554) | 1:66:A:ALA:H    | 1:64:A:LEU:HB3   | 10       | 0.97          |
| (1,1535) | 1:62:A:GLN:H    | 1:66:A:ALA:HB2   | 8        | 0.97          |
| (1,1527) | 1:66:A:ALA:HB3  | 1:68:A:VAL:H     | 5        | 0.97          |
| (1,1527) | 1:66:A:ALA:HB2  | 1:68:A:VAL:H     | 6        | 0.97          |
| (1,1430) | 1:47:A:LEU:H    | 1:64:A:LEU:HD11  | 3        | 0.97          |
| (1,1430) | 1:47:A:LEU:H    | 1:64:A:LEU:HD11  | 4        | 0.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD11  | 8        | 0.97          |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG23 | 3        | 0.97          |
| (1,1212) | 1:62:A:GLN:H     | 1:62:A:GLN:HE21  | 8        | 0.97          |
| (1,492)  | 1:122:A:THR:HG23 | 1:119:A:MET:HG2  | 5        | 0.97          |
| (1,229)  | 1:63:A:GLY:HA2   | 1:111:A:VAL:HG13 | 4        | 0.97          |
| (1,99)   | 1:38:A:SER:HB2   | 1:90:A:PRO:HG2   | 5        | 0.97          |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG2   | 6        | 0.97          |
| (1,1554) | 1:66:A:ALA:H     | 1:64:A:LEU:HB3   | 5        | 0.96          |
| (1,1554) | 1:66:A:ALA:H     | 1:58:A:PRO:HB3   | 7        | 0.96          |
| (1,1527) | 1:66:A:ALA:HB2   | 1:68:A:VAL:H     | 7        | 0.96          |
| (1,1522) | 1:105:A:ARG:HD2  | 1:102:A:SER:HA   | 9        | 0.96          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 6        | 0.96          |
| (1,1212) | 1:62:A:GLN:H     | 1:62:A:GLN:HE21  | 10       | 0.96          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG12 | 2        | 0.96          |
| (1,744)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB3   | 9        | 0.96          |
| (1,632)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HG3   | 1        | 0.96          |
| (1,1554) | 1:66:A:ALA:H     | 1:64:A:LEU:HB2   | 4        | 0.95          |
| (1,1527) | 1:66:A:ALA:HB2   | 1:68:A:VAL:H     | 4        | 0.95          |
| (1,1212) | 1:62:A:GLN:H     | 1:62:A:GLN:HE21  | 6        | 0.95          |
| (1,1186) | 1:62:A:GLN:HE22  | 1:75:A:PRO:HB2   | 8        | 0.95          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG13 | 7        | 0.95          |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 7        | 0.95          |
| (1,898)  | 1:52:A:LEU:HD22  | 1:53:A:ASP:H     | 4        | 0.95          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG22  | 2        | 0.95          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB3  | 5        | 0.95          |
| (1,301)  | 1:73:A:THR:HG22  | 1:76:A:GLU:HB3   | 4        | 0.95          |
| (1,1554) | 1:66:A:ALA:H     | 1:64:A:LEU:HB3   | 9        | 0.94          |
| (1,1527) | 1:66:A:ALA:HB3   | 1:68:A:VAL:H     | 1        | 0.94          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE1   | 4        | 0.94          |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG21 | 4        | 0.94          |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG21 | 7        | 0.94          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG12 | 8        | 0.94          |
| (1,898)  | 1:52:A:LEU:HD11  | 1:53:A:ASP:H     | 5        | 0.94          |
| (1,736)  | 1:86:A:ILE:HG21  | 1:85:A:TYR:HD2   | 7        | 0.94          |
| (1,642)  | 1:46:A:ALA:HB1   | 1:85:A:TYR:HD1   | 9        | 0.94          |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG2   | 4        | 0.94          |
| (1,1494) | 1:122:A:THR:HG21 | 1:121:A:ASP:HB3  | 3        | 0.93          |
| (1,898)  | 1:52:A:LEU:HD13  | 1:53:A:ASP:H     | 9        | 0.93          |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 9        | 0.93          |
| (1,809)  | 1:100:A:LEU:HD13 | 1:63:A:GLY:H     | 3        | 0.93          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG21  | 6        | 0.93          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 1        | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,665)  | 1:109:A:VAL:HG21 | 1:102:A:SER:HB2  | 3        | 0.93          |
| (1,1562) | 1:102:A:SER:H    | 1:109:A:VAL:HB   | 7        | 0.92          |
| (1,1527) | 1:66:A:ALA:HB2   | 1:68:A:VAL:H     | 2        | 0.92          |
| (1,1527) | 1:66:A:ALA:HB1   | 1:68:A:VAL:H     | 8        | 0.92          |
| (1,1444) | 1:27:A:ASN:HB3   | 1:28:A:LYS:HB2   | 10       | 0.92          |
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD11  | 7        | 0.92          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG13 | 1        | 0.92          |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 1        | 0.92          |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 5        | 0.92          |
| (1,898)  | 1:52:A:LEU:HD22  | 1:53:A:ASP:H     | 2        | 0.92          |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 7        | 0.92          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG22  | 9        | 0.92          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 4        | 0.92          |
| (1,666)  | 1:109:A:VAL:HG23 | 1:44:A:GLU:HG2   | 5        | 0.92          |
| (1,665)  | 1:109:A:VAL:HG23 | 1:102:A:SER:HB2  | 9        | 0.92          |
| (1,361)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HA   | 2        | 0.92          |
| (1,301)  | 1:73:A:THR:HG22  | 1:76:A:GLU:HB3   | 8        | 0.92          |
| (1,1527) | 1:66:A:ALA:HB1   | 1:68:A:VAL:H     | 9        | 0.91          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 4        | 0.91          |
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD13  | 2        | 0.91          |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG23 | 8        | 0.91          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG11 | 10       | 0.91          |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 4        | 0.91          |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 9        | 0.91          |
| (1,787)  | 1:96:A:ALA:HB3   | 1:114:A:TYR:HB3  | 4        | 0.91          |
| (1,744)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB3   | 5        | 0.91          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 9        | 0.91          |
| (1,301)  | 1:73:A:THR:HG21  | 1:76:A:GLU:HB3   | 9        | 0.91          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG22  | 8        | 0.9           |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB3   | 4        | 0.9           |
| (1,1522) | 1:105:A:ARG:HD3  | 1:106:A:HIS:HA   | 3        | 0.9           |
| (1,1417) | 1:33:A:ARG:H     | 1:116:A:PRO:HG2  | 10       | 0.9           |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 3        | 0.9           |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 10       | 0.9           |
| (1,809)  | 1:100:A:LEU:HD12 | 1:63:A:GLY:H     | 6        | 0.9           |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 10       | 0.9           |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG23  | 1        | 0.9           |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG23  | 5        | 0.9           |
| (1,744)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB3   | 10       | 0.9           |
| (1,361)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HA   | 7        | 0.9           |
| (1,99)   | 1:38:A:SER:HB2   | 1:90:A:PRO:HG2   | 2        | 0.9           |
| (1,1444) | 1:27:A:ASN:HB2   | 1:28:A:LYS:HB2   | 3        | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD13  | 6        | 0.89          |
| (1,1353) | 1:138:A:ASN:HD21 | 1:138:A:ASN:HA   | 5        | 0.89          |
| (1,898)  | 1:52:A:LEU:HD22  | 1:53:A:ASP:H     | 3        | 0.89          |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 1        | 0.89          |
| (1,736)  | 1:86:A:ILE:HG21  | 1:85:A:TYR:HD2   | 3        | 0.89          |
| (1,736)  | 1:86:A:ILE:HG21  | 1:85:A:TYR:HD1   | 5        | 0.89          |
| (1,666)  | 1:109:A:VAL:HG22 | 1:44:A:GLU:HG2   | 9        | 0.89          |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG3   | 1        | 0.89          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG23  | 5        | 0.88          |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG23 | 1        | 0.88          |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG23 | 5        | 0.88          |
| (1,1349) | 1:52:A:LEU:H     | 1:48:A:ASP:HB3   | 5        | 0.88          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG13 | 5        | 0.88          |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 6        | 0.88          |
| (1,912)  | 1:117:A:ASP:H    | 1:116:A:PRO:HG3  | 9        | 0.88          |
| (1,809)  | 1:100:A:LEU:HD12 | 1:63:A:GLY:H     | 5        | 0.88          |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD13  | 9        | 0.88          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 8        | 0.88          |
| (1,301)  | 1:73:A:THR:HG21  | 1:76:A:GLU:HB3   | 1        | 0.88          |
| (1,229)  | 1:63:A:GLY:HA2   | 1:111:A:VAL:HG13 | 8        | 0.88          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG21  | 6        | 0.87          |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG22  | 3        | 0.87          |
| (1,1524) | 1:60:A:THR:HB    | 1:100:A:LEU:HG   | 10       | 0.87          |
| (1,1444) | 1:27:A:ASN:HB2   | 1:28:A:LYS:HB2   | 5        | 0.87          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG13 | 7        | 0.87          |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 7        | 0.87          |
| (1,898)  | 1:52:A:LEU:HD23  | 1:53:A:ASP:H     | 1        | 0.87          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD11  | 3        | 0.87          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG22  | 8        | 0.87          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 3        | 0.87          |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD11  | 5        | 0.87          |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD12  | 10       | 0.87          |
| (1,361)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HA   | 6        | 0.87          |
| (1,1541) | 1:86:A:ILE:HG22  | 1:87:A:ARG:H     | 2        | 0.86          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB1   | 8        | 0.86          |
| (1,1493) | 1:109:A:VAL:HG12 | 1:108:A:LYS:H    | 7        | 0.86          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB3   | 5        | 0.86          |
| (1,898)  | 1:52:A:LEU:HD21  | 1:53:A:ASP:H     | 8        | 0.86          |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 8        | 0.86          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG23  | 7        | 0.86          |
| (1,666)  | 1:109:A:VAL:HG22 | 1:44:A:GLU:HG2   | 4        | 0.86          |
| (1,665)  | 1:109:A:VAL:HG23 | 1:102:A:SER:HB2  | 6        | 0.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG22  | 4        | 0.86          |
| (1,301)  | 1:73:A:THR:HG22  | 1:76:A:GLU:HB3   | 6        | 0.86          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG21  | 3        | 0.85          |
| (1,1535) | 1:62:A:GLN:H     | 1:66:A:ALA:HB3   | 4        | 0.85          |
| (1,1535) | 1:62:A:GLN:H     | 1:66:A:ALA:HB1   | 5        | 0.85          |
| (1,1524) | 1:60:A:THR:HB    | 1:100:A:LEU:HG   | 5        | 0.85          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB2   | 5        | 0.85          |
| (1,1430) | 1:47:A:LEU:H     | 1:64:A:LEU:HD13  | 5        | 0.85          |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 2        | 0.85          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD11  | 4        | 0.85          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 2        | 0.85          |
| (1,736)  | 1:86:A:ILE:HG23  | 1:85:A:TYR:HD1   | 1        | 0.85          |
| (1,736)  | 1:86:A:ILE:HG23  | 1:85:A:TYR:HD2   | 10       | 0.85          |
| (1,667)  | 1:109:A:VAL:HG22 | 1:108:A:LYS:HB2  | 4        | 0.85          |
| (1,661)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HG12  | 9        | 0.85          |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD11  | 4        | 0.85          |
| (1,647)  | 1:42:A:ALA:HB2   | 1:43:A:LEU:HD13  | 8        | 0.85          |
| (1,301)  | 1:73:A:THR:HG22  | 1:76:A:GLU:HB3   | 2        | 0.85          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG23  | 1        | 0.84          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG22  | 2        | 0.84          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG23  | 7        | 0.84          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB1   | 3        | 0.84          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB2   | 10       | 0.84          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE1   | 7        | 0.84          |
| (1,1524) | 1:60:A:THR:HB    | 1:101:A:VAL:HG21 | 6        | 0.84          |
| (1,1493) | 1:109:A:VAL:HG13 | 1:108:A:LYS:H    | 4        | 0.84          |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG22 | 4        | 0.84          |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 10       | 0.84          |
| (1,809)  | 1:100:A:LEU:HD11 | 1:63:A:GLY:H     | 4        | 0.84          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD11  | 8        | 0.84          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG23  | 4        | 0.84          |
| (1,647)  | 1:42:A:ALA:HB2   | 1:43:A:LEU:HD11  | 2        | 0.84          |
| (1,647)  | 1:42:A:ALA:HB2   | 1:43:A:LEU:HD11  | 7        | 0.84          |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB2   | 1        | 0.84          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG23  | 4        | 0.83          |
| (1,1515) | 1:30:A:LYS:HB3   | 1:30:A:LYS:HE2   | 6        | 0.83          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG11 | 6        | 0.83          |
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2   | 6        | 0.83          |
| (1,754)  | 1:38:A:SER:HB2   | 1:37:A:ILE:HG21  | 3        | 0.83          |
| (1,736)  | 1:86:A:ILE:HG21  | 1:85:A:TYR:HD2   | 2        | 0.83          |
| (1,666)  | 1:109:A:VAL:HG21 | 1:44:A:GLU:HG2   | 8        | 0.83          |
| (1,665)  | 1:109:A:VAL:HG22 | 1:102:A:SER:HB2  | 8        | 0.83          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,647)  | 1:42:A:ALA:HB1   | 1:43:A:LEU:HD12  | 1        | 0.83          |
| (1,647)  | 1:42:A:ALA:HB3   | 1:43:A:LEU:HD13  | 3        | 0.83          |
| (1,647)  | 1:42:A:ALA:HB2   | 1:43:A:LEU:HD11  | 6        | 0.83          |
| (1,301)  | 1:73:A:THR:HG22  | 1:76:A:GLU:HB3   | 5        | 0.83          |
| (1,301)  | 1:73:A:THR:HG23  | 1:76:A:GLU:HB3   | 10       | 0.83          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 4        | 0.83          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 9        | 0.83          |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG2   | 9        | 0.83          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB2   | 9        | 0.82          |
| (1,1524) | 1:60:A:THR:HB    | 1:100:A:LEU:HG   | 2        | 0.82          |
| (1,1524) | 1:60:A:THR:HB    | 1:100:A:LEU:HG   | 9        | 0.82          |
| (1,1522) | 1:105:A:ARG:HD3  | 1:106:A:HIS:HA   | 5        | 0.82          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 5        | 0.82          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG11  | 4        | 0.82          |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD1  | 7        | 0.82          |
| (1,655)  | 1:56:A:ARG:HB3   | 1:57:A:TYR:H     | 4        | 0.82          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 8        | 0.82          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 10       | 0.82          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB2   | 7        | 0.81          |
| (1,1524) | 1:60:A:THR:HB    | 1:101:A:VAL:HG23 | 3        | 0.81          |
| (1,1515) | 1:30:A:LYS:HB3   | 1:30:A:LYS:HE3   | 4        | 0.81          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 2        | 0.81          |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG21 | 2        | 0.81          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG11  | 5        | 0.81          |
| (1,1172) | 1:101:A:VAL:H    | 1:109:A:VAL:HG11 | 4        | 0.81          |
| (1,787)  | 1:96:A:ALA:HB2   | 1:114:A:TYR:HB3  | 6        | 0.81          |
| (1,665)  | 1:109:A:VAL:HG22 | 1:102:A:SER:HB2  | 2        | 0.81          |
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG22  | 8        | 0.81          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 5        | 0.81          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG22  | 9        | 0.8           |
| (1,1541) | 1:86:A:ILE:HG23  | 1:87:A:ARG:H     | 8        | 0.8           |
| (1,1524) | 1:60:A:THR:HB    | 1:101:A:VAL:HG23 | 1        | 0.8           |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG23 | 3        | 0.8           |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG21 | 6        | 0.8           |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG22 | 7        | 0.8           |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG12  | 3        | 0.8           |
| (1,667)  | 1:109:A:VAL:HG23 | 1:108:A:LYS:HB2  | 5        | 0.8           |
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG21  | 10       | 0.8           |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB3   | 5        | 0.8           |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB2   | 7        | 0.8           |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG3   | 7        | 0.8           |
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 6        | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB3   | 2        | 0.79          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB1   | 5        | 0.79          |
| (1,1524) | 1:60:A:THR:HB    | 1:100:A:LEU:HG   | 4        | 0.79          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 10       | 0.79          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB1   | 1        | 0.79          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB3   | 10       | 0.79          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB3   | 3        | 0.79          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD12  | 1        | 0.79          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD12  | 2        | 0.79          |
| (1,661)  | 1:111:A:VAL:HG21 | 1:40:A:ILE:HG12  | 8        | 0.79          |
| (1,619)  | 1:100:A:LEU:HD23 | 1:100:A:LEU:HA   | 1        | 0.79          |
| (1,619)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:HA   | 7        | 0.79          |
| (1,619)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:HA   | 10       | 0.79          |
| (1,281)  | 1:40:A:ILE:HD11  | 1:41:A:VAL:H     | 2        | 0.79          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 6        | 0.79          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 7        | 0.79          |
| (1,1493) | 1:109:A:VAL:HG11 | 1:108:A:LYS:H    | 2        | 0.78          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 9        | 0.78          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB2   | 8        | 0.78          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG22 | 10       | 0.78          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG11  | 2        | 0.78          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG12  | 9        | 0.78          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG13  | 10       | 0.78          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD11  | 5        | 0.78          |
| (1,619)  | 1:100:A:LEU:HD23 | 1:100:A:LEU:HA   | 6        | 0.78          |
| (1,361)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HA   | 8        | 0.78          |
| (1,301)  | 1:73:A:THR:HG21  | 1:76:A:GLU:HB3   | 3        | 0.78          |
| (1,301)  | 1:73:A:THR:HG23  | 1:76:A:GLU:HB3   | 7        | 0.78          |
| (1,281)  | 1:40:A:ILE:HD11  | 1:41:A:VAL:H     | 4        | 0.78          |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG3   | 10       | 0.78          |
| (1,1543) | 1:64:A:LEU:HD12  | 1:67:A:LEU:H     | 3        | 0.77          |
| (1,1541) | 1:86:A:ILE:HG21  | 1:87:A:ARG:H     | 10       | 0.77          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE1   | 2        | 0.77          |
| (1,1474) | 1:56:A:ARG:HD3   | 1:50:A:TYR:HE1   | 2        | 0.77          |
| (1,1303) | 1:125:A:ASP:H    | 1:122:A:THR:HG23 | 6        | 0.77          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG23 | 1        | 0.77          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG22 | 6        | 0.77          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG13 | 1        | 0.77          |
| (1,1202) | 1:48:A:ASP:H     | 1:49:A:MET:HG3   | 10       | 0.77          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG11  | 7        | 0.77          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB3   | 8        | 0.77          |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 4        | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2   | 8        | 0.77          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 8        | 0.77          |
| (1,665)  | 1:109:A:VAL:HG21 | 1:102:A:SER:HB2  | 10       | 0.77          |
| (1,655)  | 1:56:A:ARG:HB3   | 1:57:A:TYR:H     | 2        | 0.77          |
| (1,619)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:HA   | 3        | 0.77          |
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG23  | 9        | 0.77          |
| (1,281)  | 1:40:A:ILE:HD13  | 1:41:A:VAL:H     | 8        | 0.77          |
| (1,1566) | 1:40:A:ILE:H     | 1:37:A:ILE:HG22  | 10       | 0.76          |
| (1,1524) | 1:60:A:THR:HB    | 1:100:A:LEU:HG   | 8        | 0.76          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 7        | 0.76          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB3   | 7        | 0.76          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB3   | 9        | 0.76          |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG23 | 10       | 0.76          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 4        | 0.76          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG12  | 6        | 0.76          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG12  | 8        | 0.76          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB1   | 6        | 0.76          |
| (1,665)  | 1:109:A:VAL:HG22 | 1:102:A:SER:HB2  | 1        | 0.76          |
| (1,661)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HG12  | 5        | 0.76          |
| (1,619)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:HA   | 9        | 0.76          |
| (1,361)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HA   | 4        | 0.76          |
| (1,281)  | 1:40:A:ILE:HD12  | 1:41:A:VAL:H     | 7        | 0.76          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB2   | 6        | 0.75          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 8        | 0.75          |
| (1,1312) | 1:86:A:ILE:H     | 1:83:A:ASP:HB3   | 8        | 0.75          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG13 | 3        | 0.75          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD21  | 1        | 0.75          |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD12  | 6        | 0.75          |
| (1,737)  | 1:40:A:ILE:HD12  | 1:128:A:ASN:H    | 8        | 0.75          |
| (1,665)  | 1:109:A:VAL:HG21 | 1:102:A:SER:HB2  | 5        | 0.75          |
| (1,665)  | 1:109:A:VAL:HG22 | 1:102:A:SER:HB2  | 7        | 0.75          |
| (1,642)  | 1:46:A:ALA:HB3   | 1:85:A:TYR:HD2   | 8        | 0.75          |
| (1,619)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:HA   | 5        | 0.75          |
| (1,619)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:HA   | 8        | 0.75          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 2        | 0.75          |
| (1,281)  | 1:40:A:ILE:HD11  | 1:41:A:VAL:H     | 3        | 0.75          |
| (1,281)  | 1:40:A:ILE:HD13  | 1:41:A:VAL:H     | 5        | 0.75          |
| (1,281)  | 1:40:A:ILE:HD12  | 1:41:A:VAL:H     | 9        | 0.75          |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 5        | 0.75          |
| (1,1541) | 1:86:A:ILE:HG22  | 1:87:A:ARG:H     | 7        | 0.74          |
| (1,1531) | 1:44:A:GLU:H     | 1:46:A:ALA:HB3   | 1        | 0.74          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 6        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB1   | 2        | 0.74          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB2   | 3        | 0.74          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 4        | 0.74          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB2   | 1        | 0.74          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB1   | 9        | 0.74          |
| (1,661)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HG12  | 10       | 0.74          |
| (1,619)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:HA   | 2        | 0.74          |
| (1,619)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:HA   | 4        | 0.74          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 5        | 0.74          |
| (1,361)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HA   | 3        | 0.74          |
| (1,359)  | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 6        | 0.74          |
| (1,281)  | 1:40:A:ILE:HD11  | 1:41:A:VAL:H     | 1        | 0.74          |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB2   | 10       | 0.74          |
| (1,1524) | 1:60:A:THR:HB    | 1:101:A:VAL:HG22 | 7        | 0.73          |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 1        | 0.73          |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG21 | 8        | 0.73          |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 1        | 0.73          |
| (1,737)  | 1:40:A:ILE:HD12  | 1:128:A:ASN:H    | 1        | 0.73          |
| (1,737)  | 1:40:A:ILE:HD13  | 1:128:A:ASN:H    | 4        | 0.73          |
| (1,665)  | 1:109:A:VAL:HG23 | 1:102:A:SER:HB2  | 4        | 0.73          |
| (1,661)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HG12  | 4        | 0.73          |
| (1,468)  | 1:44:A:GLU:HG2   | 1:40:A:ILE:HG23  | 5        | 0.73          |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG23  | 6        | 0.73          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 3        | 0.73          |
| (1,281)  | 1:40:A:ILE:HD11  | 1:41:A:VAL:H     | 10       | 0.73          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 1        | 0.73          |
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 7        | 0.72          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB3   | 6        | 0.72          |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG23 | 2        | 0.72          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 1        | 0.72          |
| (1,796)  | 1:121:A:ASP:HB3  | 1:120:A:PRO:HB2  | 3        | 0.72          |
| (1,787)  | 1:96:A:ALA:HB3   | 1:114:A:TYR:HB3  | 5        | 0.72          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 7        | 0.72          |
| (1,359)  | 1:64:A:LEU:HD12  | 1:67:A:LEU:H     | 3        | 0.72          |
| (1,281)  | 1:40:A:ILE:HD13  | 1:41:A:VAL:H     | 6        | 0.72          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 3        | 0.72          |
| (1,183)  | 1:32:A:ASP:HB3   | 1:28:A:LYS:HG3   | 2        | 0.72          |
| (1,93)   | 1:37:A:ILE:HG21  | 1:132:A:GLY:HA2  | 9        | 0.72          |
| (1,1575) | 1:118:A:GLY:H    | 1:114:A:TYR:HD1  | 7        | 0.71          |
| (1,1541) | 1:86:A:ILE:HG22  | 1:87:A:ARG:H     | 3        | 0.71          |
| (1,1463) | 1:45:A:SER:HB3   | 1:46:A:ALA:HB1   | 4        | 0.71          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 3        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1047) | 1:56:A:ARG:H     | 1:56:A:ARG:HG2   | 9        | 0.71          |
| (1,737)  | 1:40:A:ILE:HD12  | 1:128:A:ASN:H    | 3        | 0.71          |
| (1,641)  | 1:46:A:ALA:HB3   | 1:45:A:SER:H     | 4        | 0.71          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 7        | 0.71          |
| (1,230)  | 1:63:A:GLY:HA2   | 1:65:A:GLY:H     | 2        | 0.71          |
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 5        | 0.7           |
| (1,1498) | 1:57:A:TYR:HE2   | 1:47:A:LEU:HG    | 6        | 0.7           |
| (1,1467) | 1:65:A:GLY:HA3   | 1:69:A:LYS:H     | 3        | 0.7           |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 4        | 0.7           |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE2   | 1        | 0.7           |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB2   | 2        | 0.7           |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 3        | 0.7           |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 5        | 0.7           |
| (1,785)  | 1:53:A:ASP:HA    | 1:52:A:LEU:HD13  | 9        | 0.7           |
| (1,361)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HA   | 5        | 0.7           |
| (1,338)  | 1:52:A:LEU:HD22  | 1:52:A:LEU:H     | 10       | 0.7           |
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 2        | 0.69          |
| (1,1503) | 1:89:A:LEU:HB2   | 1:88:A:ARG:HA    | 2        | 0.69          |
| (1,1498) | 1:57:A:TYR:HE2   | 1:47:A:LEU:HG    | 3        | 0.69          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB2   | 10       | 0.69          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB1   | 6        | 0.69          |
| (1,1183) | 1:44:A:GLU:H     | 1:41:A:VAL:HG12  | 1        | 0.69          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG23  | 5        | 0.69          |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 2        | 0.69          |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 7        | 0.69          |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 10       | 0.69          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 5        | 0.69          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 3        | 0.69          |
| (1,93)   | 1:37:A:ILE:HG22  | 1:132:A:GLY:HA2  | 5        | 0.69          |
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 4        | 0.68          |
| (1,1541) | 1:86:A:ILE:HG21  | 1:87:A:ARG:H     | 1        | 0.68          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD23  | 3        | 0.68          |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 9        | 0.68          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 6        | 0.68          |
| (1,826)  | 1:35:A:LYS:H     | 1:35:A:LYS:HD3   | 8        | 0.68          |
| (1,737)  | 1:40:A:ILE:HD12  | 1:128:A:ASN:H    | 2        | 0.68          |
| (1,737)  | 1:40:A:ILE:HD13  | 1:128:A:ASN:H    | 7        | 0.68          |
| (1,661)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HG12  | 1        | 0.68          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 9        | 0.68          |
| (1,361)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HA   | 10       | 0.68          |
| (1,358)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HB3  | 10       | 0.68          |
| (1,99)   | 1:38:A:SER:HB3   | 1:90:A:PRO:HG2   | 3        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1543) | 1:64:A:LEU:HD12  | 1:67:A:LEU:H     | 8        | 0.67          |
| (1,1494) | 1:122:A:THR:HG23 | 1:121:A:ASP:HB3  | 6        | 0.67          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 6        | 0.67          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG11 | 6        | 0.67          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG22 | 3        | 0.67          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 5        | 0.67          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 7        | 0.67          |
| (1,1047) | 1:56:A:ARG:H     | 1:56:A:ARG:HG2   | 3        | 0.67          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG22  | 8        | 0.67          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG22  | 9        | 0.67          |
| (1,845)  | 1:80:A:TYR:H     | 1:80:A:TYR:HB2   | 6        | 0.67          |
| (1,737)  | 1:40:A:ILE:HD11  | 1:128:A:ASN:H    | 6        | 0.67          |
| (1,737)  | 1:40:A:ILE:HD13  | 1:128:A:ASN:H    | 9        | 0.67          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 6        | 0.67          |
| (1,661)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HG12  | 2        | 0.67          |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG22  | 3        | 0.67          |
| (1,449)  | 1:109:A:VAL:HG13 | 1:108:A:LYS:HD3  | 9        | 0.67          |
| (1,361)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HA   | 1        | 0.67          |
| (1,359)  | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 7        | 0.67          |
| (1,334)  | 1:52:A:LEU:HD22  | 1:51:A:LYS:HG2   | 10       | 0.67          |
| (1,194)  | 1:111:A:VAL:HG13 | 1:43:A:LEU:HD11  | 1        | 0.67          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD13  | 4        | 0.67          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD13  | 5        | 0.67          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD1   | 5        | 0.67          |
| (1,1541) | 1:86:A:ILE:HG21  | 1:87:A:ARG:H     | 4        | 0.66          |
| (1,1503) | 1:126:A:ILE:HB   | 1:113:A:SER:HA   | 3        | 0.66          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 10       | 0.66          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 1        | 0.66          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 2        | 0.66          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 3        | 0.66          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 6        | 0.66          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG22  | 4        | 0.66          |
| (1,766)  | 1:131:A:VAL:HG21 | 1:128:A:ASN:HB3  | 8        | 0.66          |
| (1,737)  | 1:40:A:ILE:HD11  | 1:128:A:ASN:H    | 5        | 0.66          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 5        | 0.66          |
| (1,699)  | 1:101:A:VAL:HG23 | 1:105:A:ARG:HD3  | 7        | 0.66          |
| (1,666)  | 1:109:A:VAL:HG23 | 1:44:A:GLU:HG2   | 10       | 0.66          |
| (1,661)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HG12  | 7        | 0.66          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD13 | 3        | 0.66          |
| (1,93)   | 1:37:A:ILE:HG21  | 1:132:A:GLY:HA2  | 2        | 0.66          |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG23  | 6        | 0.65          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB2   | 4        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1541) | 1:86:A:ILE:HG22  | 1:87:A:ARG:H     | 5        | 0.65          |
| (1,1525) | 1:75:A:PRO:HG3   | 1:50:A:TYR:HE2   | 9        | 0.65          |
| (1,1446) | 1:31:A:ALA:HB3   | 1:30:A:LYS:HB3   | 3        | 0.65          |
| (1,1375) | 1:99:A:GLN:H     | 1:111:A:VAL:HG23 | 9        | 0.65          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD23  | 9        | 0.65          |
| (1,1047) | 1:56:A:ARG:H     | 1:56:A:ARG:HG2   | 6        | 0.65          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB1   | 7        | 0.65          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG21  | 1        | 0.65          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG22  | 2        | 0.65          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG22  | 10       | 0.65          |
| (1,765)  | 1:37:A:ILE:HD11  | 1:33:A:ARG:H     | 2        | 0.65          |
| (1,737)  | 1:40:A:ILE:HD12  | 1:128:A:ASN:H    | 10       | 0.65          |
| (1,661)  | 1:111:A:VAL:HG21 | 1:40:A:ILE:HG12  | 6        | 0.65          |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD23  | 9        | 0.65          |
| (1,359)  | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 5        | 0.65          |
| (1,358)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HB3  | 7        | 0.65          |
| (1,338)  | 1:52:A:LEU:HD22  | 1:52:A:LEU:H     | 7        | 0.65          |
| (1,93)   | 1:37:A:ILE:HG21  | 1:132:A:GLY:HA2  | 8        | 0.65          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB2   | 2        | 0.64          |
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 1        | 0.64          |
| (1,1541) | 1:86:A:ILE:HG22  | 1:87:A:ARG:H     | 6        | 0.64          |
| (1,1494) | 1:122:A:THR:HG23 | 1:121:A:ASP:HB3  | 10       | 0.64          |
| (1,1491) | 1:43:A:LEU:HD13  | 1:39:A:ASP:HA    | 9        | 0.64          |
| (1,1446) | 1:31:A:ALA:HB1   | 1:30:A:LYS:HB3   | 5        | 0.64          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE1   | 1        | 0.64          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 8        | 0.64          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB1   | 10       | 0.64          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 8        | 0.64          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG23  | 3        | 0.64          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG23  | 7        | 0.64          |
| (1,765)  | 1:37:A:ILE:HD12  | 1:33:A:ARG:H     | 1        | 0.64          |
| (1,765)  | 1:37:A:ILE:HD13  | 1:33:A:ARG:H     | 7        | 0.64          |
| (1,655)  | 1:56:A:ARG:HB3   | 1:57:A:TYR:H     | 8        | 0.64          |
| (1,641)  | 1:46:A:ALA:HB2   | 1:45:A:SER:H     | 10       | 0.64          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 4        | 0.64          |
| (1,395)  | 1:97:A:GLU:HB2   | 1:97:A:GLU:H     | 3        | 0.64          |
| (1,395)  | 1:97:A:GLU:HB2   | 1:97:A:GLU:H     | 7        | 0.64          |
| (1,360)  | 1:64:A:LEU:HD12  | 1:68:A:VAL:H     | 1        | 0.64          |
| (1,359)  | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 2        | 0.64          |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB3   | 2        | 0.64          |
| (1,93)   | 1:37:A:ILE:HG22  | 1:132:A:GLY:HA2  | 1        | 0.64          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB2   | 6        | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB1   | 8        | 0.63          |
| (1,1493) | 1:109:A:VAL:HG12 | 1:108:A:LYS:H    | 1        | 0.63          |
| (1,1474) | 1:56:A:ARG:HD2   | 1:50:A:TYR:HE2   | 9        | 0.63          |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE2   | 7        | 0.63          |
| (1,1250) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HG2  | 1        | 0.63          |
| (1,1171) | 1:100:A:LEU:HD23 | 1:101:A:VAL:H    | 4        | 0.63          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 10       | 0.63          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB1   | 3        | 0.63          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB1   | 5        | 0.63          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB1   | 10       | 0.63          |
| (1,765)  | 1:37:A:ILE:HD12  | 1:33:A:ARG:H     | 10       | 0.63          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 2        | 0.63          |
| (1,717)  | 1:65:A:GLY:HA3   | 1:68:A:VAL:HB    | 10       | 0.63          |
| (1,686)  | 1:98:A:TYR:HB2   | 1:64:A:LEU:HD21  | 1        | 0.63          |
| (1,667)  | 1:109:A:VAL:HG22 | 1:108:A:LYS:HB2  | 6        | 0.63          |
| (1,642)  | 1:46:A:ALA:HB1   | 1:85:A:TYR:HD1   | 10       | 0.63          |
| (1,641)  | 1:46:A:ALA:HB3   | 1:45:A:SER:H     | 2        | 0.63          |
| (1,641)  | 1:46:A:ALA:HB1   | 1:45:A:SER:H     | 8        | 0.63          |
| (1,641)  | 1:46:A:ALA:HB2   | 1:45:A:SER:H     | 9        | 0.63          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 2        | 0.63          |
| (1,359)  | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 4        | 0.63          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD12  | 9        | 0.63          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD11  | 10       | 0.63          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB3   | 1        | 0.62          |
| (1,1503) | 1:89:A:LEU:HB2   | 1:88:A:ARG:HA    | 9        | 0.62          |
| (1,1493) | 1:109:A:VAL:HG12 | 1:108:A:LYS:H    | 5        | 0.62          |
| (1,1493) | 1:109:A:VAL:HG13 | 1:108:A:LYS:H    | 6        | 0.62          |
| (1,1491) | 1:43:A:LEU:HD12  | 1:39:A:ASP:HA    | 1        | 0.62          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 10       | 0.62          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 2        | 0.62          |
| (1,1317) | 1:97:A:GLU:HA    | 1:91:A:GLN:HE21  | 9        | 0.62          |
| (1,1262) | 1:134:A:SER:H    | 1:132:A:GLY:HA3  | 10       | 0.62          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG12 | 4        | 0.62          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB1   | 4        | 0.62          |
| (1,1085) | 1:100:A:LEU:HB3  | 1:101:A:VAL:H    | 9        | 0.62          |
| (1,1047) | 1:56:A:ARG:H     | 1:56:A:ARG:HG2   | 7        | 0.62          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 7        | 0.62          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB1   | 4        | 0.62          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB1   | 9        | 0.62          |
| (1,857)  | 1:60:A:THR:H     | 1:60:A:THR:HG21  | 6        | 0.62          |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 10       | 0.62          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB2  | 7        | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,641)  | 1:46:A:ALA:HB1   | 1:45:A:SER:H     | 3        | 0.62          |
| (1,641)  | 1:46:A:ALA:HB2   | 1:45:A:SER:H     | 6        | 0.62          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD12 | 5        | 0.62          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 7        | 0.62          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 10       | 0.62          |
| (1,488)  | 1:59:A:THR:HG22  | 1:62:A:GLN:H     | 9        | 0.62          |
| (1,451)  | 1:109:A:VAL:HG11 | 1:100:A:LEU:HD13 | 3        | 0.62          |
| (1,359)  | 1:64:A:LEU:HD12  | 1:67:A:LEU:H     | 8        | 0.62          |
| (1,87)   | 1:37:A:ILE:HD11  | 1:126:A:ILE:HA   | 3        | 0.62          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB3   | 5        | 0.61          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB2   | 7        | 0.61          |
| (1,1515) | 1:28:A:LYS:HB3   | 1:28:A:LYS:HE3   | 1        | 0.61          |
| (1,1492) | 1:43:A:LEU:HD12  | 1:43:A:LEU:H     | 3        | 0.61          |
| (1,1492) | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 4        | 0.61          |
| (1,1492) | 1:43:A:LEU:HD12  | 1:43:A:LEU:H     | 8        | 0.61          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 4        | 0.61          |
| (1,1340) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD22 | 4        | 0.61          |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD13  | 8        | 0.61          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG22 | 5        | 0.61          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG11 | 10       | 0.61          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD21  | 5        | 0.61          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 1        | 0.61          |
| (1,929)  | 1:49:A:MET:H     | 1:46:A:ALA:HB2   | 4        | 0.61          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 2        | 0.61          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 4        | 0.61          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 9        | 0.61          |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 6        | 0.61          |
| (1,765)  | 1:37:A:ILE:HD13  | 1:33:A:ARG:H     | 3        | 0.61          |
| (1,765)  | 1:37:A:ILE:HD11  | 1:33:A:ARG:H     | 6        | 0.61          |
| (1,642)  | 1:46:A:ALA:HB1   | 1:85:A:TYR:HD1   | 7        | 0.61          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 1        | 0.61          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 8        | 0.61          |
| (1,488)  | 1:59:A:THR:HG23  | 1:62:A:GLN:H     | 1        | 0.61          |
| (1,488)  | 1:59:A:THR:HG21  | 1:62:A:GLN:H     | 3        | 0.61          |
| (1,334)  | 1:52:A:LEU:HD22  | 1:51:A:LYS:HG2   | 7        | 0.61          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD13  | 2        | 0.61          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD12  | 8        | 0.61          |
| (1,87)   | 1:37:A:ILE:HD13  | 1:126:A:ILE:HA   | 6        | 0.61          |
| (1,1493) | 1:109:A:VAL:HG13 | 1:108:A:LYS:H    | 10       | 0.6           |
| (1,1492) | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 6        | 0.6           |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 6        | 0.6           |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 8        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 7        | 0.6           |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD13  | 4        | 0.6           |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD12  | 9        | 0.6           |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD22  | 2        | 0.6           |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD21  | 10       | 0.6           |
| (1,1147) | 1:101:A:VAL:HG22 | 1:105:A:ARG:H    | 6        | 0.6           |
| (1,1014) | 1:109:A:VAL:HG13 | 1:110:A:ASP:H    | 3        | 0.6           |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 1        | 0.6           |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 3        | 0.6           |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB3   | 2        | 0.6           |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB3   | 6        | 0.6           |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 2        | 0.6           |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 4        | 0.6           |
| (1,642)  | 1:46:A:ALA:HB2   | 1:85:A:TYR:HD1   | 4        | 0.6           |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD12 | 6        | 0.6           |
| (1,488)  | 1:59:A:THR:HG22  | 1:62:A:GLN:H     | 4        | 0.6           |
| (1,488)  | 1:59:A:THR:HG22  | 1:62:A:GLN:H     | 8        | 0.6           |
| (1,93)   | 1:37:A:ILE:HG22  | 1:132:A:GLY:HA2  | 7        | 0.6           |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD1   | 6        | 0.6           |
| (1,1503) | 1:126:A:ILE:HB   | 1:113:A:SER:HA   | 4        | 0.59          |
| (1,1492) | 1:43:A:LEU:HD11  | 1:43:A:LEU:H     | 1        | 0.59          |
| (1,1492) | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 2        | 0.59          |
| (1,1492) | 1:43:A:LEU:HD11  | 1:43:A:LEU:H     | 10       | 0.59          |
| (1,1446) | 1:31:A:ALA:HB2   | 1:28:A:LYS:HB2   | 8        | 0.59          |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 3        | 0.59          |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 5        | 0.59          |
| (1,1340) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD22 | 6        | 0.59          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG12 | 9        | 0.59          |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD3   | 4        | 0.59          |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD2   | 9        | 0.59          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG3   | 3        | 0.59          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 1        | 0.59          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB2   | 1        | 0.59          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB3   | 7        | 0.59          |
| (1,641)  | 1:46:A:ALA:HB3   | 1:45:A:SER:H     | 1        | 0.59          |
| (1,641)  | 1:46:A:ALA:HB2   | 1:45:A:SER:H     | 7        | 0.59          |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD23  | 5        | 0.59          |
| (1,488)  | 1:59:A:THR:HG23  | 1:62:A:GLN:H     | 5        | 0.59          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 4        | 0.59          |
| (1,359)  | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 1        | 0.59          |
| (1,93)   | 1:37:A:ILE:HG23  | 1:132:A:GLY:HA2  | 3        | 0.59          |
| (1,52)   | 1:33:A:ARG:HD3   | 1:37:A:ILE:HD11  | 9        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB1   | 3        | 0.58          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB1   | 9        | 0.58          |
| (1,1474) | 1:56:A:ARG:HD3   | 1:50:A:TYR:HE1   | 4        | 0.58          |
| (1,1446) | 1:31:A:ALA:HB3   | 1:30:A:LYS:HB3   | 2        | 0.58          |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 1        | 0.58          |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 7        | 0.58          |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 8        | 0.58          |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 9        | 0.58          |
| (1,1340) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD22 | 5        | 0.58          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 1        | 0.58          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG13 | 2        | 0.58          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 2        | 0.58          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD23  | 7        | 0.58          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 1        | 0.58          |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD2   | 5        | 0.58          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 10       | 0.58          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 5        | 0.58          |
| (1,921)  | 1:88:A:ARG:H     | 1:86:A:ILE:HG12  | 10       | 0.58          |
| (1,826)  | 1:35:A:LYS:H     | 1:35:A:LYS:HD3   | 1        | 0.58          |
| (1,826)  | 1:35:A:LYS:H     | 1:35:A:LYS:HD3   | 7        | 0.58          |
| (1,765)  | 1:37:A:ILE:HD12  | 1:33:A:ARG:H     | 5        | 0.58          |
| (1,765)  | 1:37:A:ILE:HD12  | 1:33:A:ARG:H     | 8        | 0.58          |
| (1,765)  | 1:37:A:ILE:HD12  | 1:33:A:ARG:H     | 9        | 0.58          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 10       | 0.58          |
| (1,736)  | 1:86:A:ILE:HG22  | 1:85:A:TYR:HD1   | 8        | 0.58          |
| (1,699)  | 1:101:A:VAL:HG23 | 1:105:A:ARG:HD3  | 9        | 0.58          |
| (1,642)  | 1:46:A:ALA:HB2   | 1:85:A:TYR:HD2   | 1        | 0.58          |
| (1,642)  | 1:46:A:ALA:HB3   | 1:85:A:TYR:HD2   | 5        | 0.58          |
| (1,510)  | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD11 | 4        | 0.58          |
| (1,488)  | 1:59:A:THR:HG23  | 1:62:A:GLN:H     | 2        | 0.58          |
| (1,488)  | 1:59:A:THR:HG22  | 1:62:A:GLN:H     | 6        | 0.58          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 1        | 0.58          |
| (1,449)  | 1:109:A:VAL:HG12 | 1:108:A:LYS:HD3  | 3        | 0.58          |
| (1,358)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HB3  | 2        | 0.58          |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 1        | 0.58          |
| (1,87)   | 1:37:A:ILE:HD13  | 1:126:A:ILE:HA   | 1        | 0.58          |
| (1,87)   | 1:37:A:ILE:HD13  | 1:126:A:ILE:HA   | 5        | 0.58          |
| (1,87)   | 1:37:A:ILE:HD13  | 1:126:A:ILE:HA   | 8        | 0.58          |
| (1,52)   | 1:33:A:ARG:HD3   | 1:37:A:ILE:HD13  | 2        | 0.58          |
| (1,1541) | 1:86:A:ILE:HG21  | 1:87:A:ARG:H     | 9        | 0.57          |
| (1,1494) | 1:122:A:THR:HG22 | 1:121:A:ASP:HB3  | 1        | 0.57          |
| (1,1492) | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 7        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1474) | 1:56:A:ARG:HD2   | 1:50:A:TYR:HE1   | 3        | 0.57          |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD12  | 2        | 0.57          |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 2        | 0.57          |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE2   | 6        | 0.57          |
| (1,1147) | 1:101:A:VAL:HG23 | 1:105:A:ARG:H    | 4        | 0.57          |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 3        | 0.57          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 8        | 0.57          |
| (1,787)  | 1:96:A:ALA:HB1   | 1:114:A:TYR:HB3  | 2        | 0.57          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 8        | 0.57          |
| (1,641)  | 1:46:A:ALA:HB1   | 1:45:A:SER:H     | 5        | 0.57          |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD23  | 2        | 0.57          |
| (1,488)  | 1:59:A:THR:HG21  | 1:62:A:GLN:H     | 10       | 0.57          |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG23  | 7        | 0.57          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 6        | 0.57          |
| (1,194)  | 1:111:A:VAL:HG12 | 1:43:A:LEU:HD12  | 3        | 0.57          |
| (1,134)  | 1:122:A:THR:HG22 | 1:123:A:ASP:H    | 2        | 0.57          |
| (1,132)  | 1:41:A:VAL:HG23  | 1:45:A:SER:HB2   | 3        | 0.57          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD2   | 3        | 0.57          |
| (1,1523) | 1:140:A:SER:HB2  | 1:139:A:GLY:H    | 6        | 0.56          |
| (1,1494) | 1:122:A:THR:HG21 | 1:121:A:ASP:HB3  | 2        | 0.56          |
| (1,1493) | 1:109:A:VAL:HG11 | 1:108:A:LYS:H    | 8        | 0.56          |
| (1,1493) | 1:109:A:VAL:HG13 | 1:108:A:LYS:H    | 9        | 0.56          |
| (1,1491) | 1:43:A:LEU:HD11  | 1:39:A:ASP:HA    | 7        | 0.56          |
| (1,1445) | 1:128:A:ASN:HA   | 1:128:A:ASN:HD22 | 2        | 0.56          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 5        | 0.56          |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD12  | 10       | 0.56          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB2   | 5        | 0.56          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB3   | 7        | 0.56          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 5        | 0.56          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB3   | 1        | 0.56          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD22  | 6        | 0.56          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG23 | 5        | 0.56          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG22 | 10       | 0.56          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 6        | 0.56          |
| (1,1014) | 1:109:A:VAL:HG12 | 1:110:A:ASP:H    | 8        | 0.56          |
| (1,720)  | 1:108:A:LYS:HA   | 1:103:A:PRO:HB2  | 2        | 0.56          |
| (1,661)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HG12  | 3        | 0.56          |
| (1,586)  | 1:48:A:ASP:HB2   | 1:48:A:ASP:H     | 5        | 0.56          |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 3        | 0.56          |
| (1,451)  | 1:109:A:VAL:HG13 | 1:100:A:LEU:HD11 | 8        | 0.56          |
| (1,449)  | 1:109:A:VAL:HG11 | 1:108:A:LYS:HD3  | 8        | 0.56          |
| (1,361)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HA   | 9        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,360)  | 1:64:A:LEU:HD12  | 1:68:A:VAL:H     | 10       | 0.56          |
| (1,212)  | 1:83:A:ASP:HB3   | 1:83:A:ASP:H     | 8        | 0.56          |
| (1,196)  | 1:111:A:VAL:HG12 | 1:44:A:GLU:HB2   | 3        | 0.56          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 4        | 0.56          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 8        | 0.56          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD13  | 6        | 0.56          |
| (1,194)  | 1:111:A:VAL:HG11 | 1:43:A:LEU:HD13  | 7        | 0.56          |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 3        | 0.56          |
| (1,93)   | 1:37:A:ILE:HG22  | 1:132:A:GLY:HA2  | 4        | 0.56          |
| (1,87)   | 1:37:A:ILE:HD12  | 1:126:A:ILE:HA   | 4        | 0.56          |
| (1,87)   | 1:37:A:ILE:HD11  | 1:126:A:ILE:HA   | 7        | 0.56          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD2   | 4        | 0.56          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD12  | 2        | 0.55          |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD2   | 2        | 0.55          |
| (1,1523) | 1:140:A:SER:HB3  | 1:139:A:GLY:H    | 5        | 0.55          |
| (1,1522) | 1:105:A:ARG:HD2  | 1:106:A:HIS:HA   | 4        | 0.55          |
| (1,1506) | 1:66:A:ALA:HB2   | 1:71:A:PRO:HB2   | 8        | 0.55          |
| (1,1492) | 1:43:A:LEU:HD12  | 1:99:A:GLN:H     | 5        | 0.55          |
| (1,1491) | 1:43:A:LEU:HD13  | 1:39:A:ASP:HA    | 3        | 0.55          |
| (1,1491) | 1:43:A:LEU:HD11  | 1:39:A:ASP:HA    | 5        | 0.55          |
| (1,1491) | 1:43:A:LEU:HD13  | 1:39:A:ASP:HA    | 8        | 0.55          |
| (1,1491) | 1:43:A:LEU:HD12  | 1:39:A:ASP:HA    | 10       | 0.55          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 9        | 0.55          |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD11  | 3        | 0.55          |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD12  | 5        | 0.55          |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD12  | 6        | 0.55          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 8        | 0.55          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD12  | 8        | 0.55          |
| (1,972)  | 1:34:A:GLN:HE21  | 1:37:A:ILE:HD11  | 10       | 0.55          |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 10       | 0.55          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 1        | 0.55          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 3        | 0.55          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 10       | 0.55          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 5        | 0.55          |
| (1,451)  | 1:109:A:VAL:HG12 | 1:100:A:LEU:HD11 | 9        | 0.55          |
| (1,196)  | 1:111:A:VAL:HG13 | 1:44:A:GLU:HB2   | 1        | 0.55          |
| (1,132)  | 1:41:A:VAL:HG22  | 1:45:A:SER:HB2   | 7        | 0.55          |
| (1,93)   | 1:37:A:ILE:HG23  | 1:132:A:GLY:HA2  | 6        | 0.55          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD2   | 2        | 0.55          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD2   | 7        | 0.55          |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD1   | 6        | 0.54          |
| (1,1503) | 1:126:A:ILE:HB   | 1:113:A:SER:HA   | 10       | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1498) | 1:57:A:TYR:HE2   | 1:47:A:LEU:HG    | 2        | 0.54          |
| (1,1491) | 1:43:A:LEU:HD11  | 1:39:A:ASP:HA    | 4        | 0.54          |
| (1,1446) | 1:31:A:ALA:HB3   | 1:30:A:LYS:HB3   | 7        | 0.54          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 1        | 0.54          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB2   | 1        | 0.54          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB3   | 4        | 0.54          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB2   | 8        | 0.54          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB2   | 10       | 0.54          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD22  | 4        | 0.54          |
| (1,1147) | 1:101:A:VAL:HG21 | 1:105:A:ARG:H    | 3        | 0.54          |
| (1,1147) | 1:101:A:VAL:HG22 | 1:105:A:ARG:H    | 10       | 0.54          |
| (1,1014) | 1:109:A:VAL:HG11 | 1:110:A:ASP:H    | 9        | 0.54          |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 1        | 0.54          |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 7        | 0.54          |
| (1,512)  | 1:91:A:GLN:HB2   | 1:92:A:ASP:H     | 8        | 0.54          |
| (1,488)  | 1:59:A:THR:HG21  | 1:62:A:GLN:H     | 7        | 0.54          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 10       | 0.54          |
| (1,449)  | 1:109:A:VAL:HG13 | 1:108:A:LYS:HD3  | 4        | 0.54          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG11  | 5        | 0.54          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG12  | 6        | 0.54          |
| (1,358)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HB3  | 9        | 0.54          |
| (1,132)  | 1:41:A:VAL:HG22  | 1:45:A:SER:HB2   | 4        | 0.54          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD1   | 1        | 0.54          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD2   | 10       | 0.54          |
| (1,1555) | 1:65:A:GLY:H     | 1:66:A:ALA:HB2   | 10       | 0.53          |
| (1,1503) | 1:89:A:LEU:HB2   | 1:88:A:ARG:HA    | 1        | 0.53          |
| (1,1498) | 1:57:A:TYR:HE2   | 1:47:A:LEU:HG    | 7        | 0.53          |
| (1,1474) | 1:56:A:ARG:HD2   | 1:50:A:TYR:HE2   | 6        | 0.53          |
| (1,1473) | 1:78:A:ARG:HD2   | 1:78:A:ARG:H     | 9        | 0.53          |
| (1,1446) | 1:31:A:ALA:HB1   | 1:30:A:LYS:HB3   | 10       | 0.53          |
| (1,1445) | 1:128:A:ASN:HA   | 1:133:A:THR:H    | 10       | 0.53          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB2   | 1        | 0.53          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG22  | 10       | 0.53          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 9        | 0.53          |
| (1,1262) | 1:134:A:SER:H    | 1:132:A:GLY:HA3  | 4        | 0.53          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB3   | 10       | 0.53          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG23 | 2        | 0.53          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG23 | 8        | 0.53          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 10       | 0.53          |
| (1,1147) | 1:101:A:VAL:HG21 | 1:105:A:ARG:H    | 5        | 0.53          |
| (1,1014) | 1:109:A:VAL:HG12 | 1:110:A:ASP:H    | 2        | 0.53          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 6        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 3        | 0.53          |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 5        | 0.53          |
| (1,765)  | 1:37:A:ILE:HD11  | 1:33:A:ARG:H     | 4        | 0.53          |
| (1,655)  | 1:56:A:ARG:HB3   | 1:57:A:TYR:H     | 5        | 0.53          |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG22  | 1        | 0.53          |
| (1,449)  | 1:109:A:VAL:HG11 | 1:108:A:LYS:HD3  | 2        | 0.53          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 6        | 0.53          |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB3  | 8        | 0.53          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 7        | 0.53          |
| (1,87)   | 1:37:A:ILE:HD12  | 1:126:A:ILE:HA   | 2        | 0.53          |
| (1,87)   | 1:37:A:ILE:HD13  | 1:126:A:ILE:HA   | 9        | 0.53          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 3        | 0.52          |
| (1,1543) | 1:64:A:LEU:HD12  | 1:67:A:LEU:H     | 10       | 0.52          |
| (1,1498) | 1:57:A:TYR:HE2   | 1:47:A:LEU:HG    | 8        | 0.52          |
| (1,1493) | 1:109:A:VAL:HG12 | 1:108:A:LYS:H    | 3        | 0.52          |
| (1,1491) | 1:43:A:LEU:HD11  | 1:39:A:ASP:HA    | 6        | 0.52          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 8        | 0.52          |
| (1,1340) | 1:109:A:VAL:HG11 | 1:128:A:ASN:HD22 | 8        | 0.52          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 9        | 0.52          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB2   | 5        | 0.52          |
| (1,1209) | 1:41:A:VAL:H     | 1:43:A:LEU:HD21  | 8        | 0.52          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD12  | 6        | 0.52          |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD3   | 6        | 0.52          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 9        | 0.52          |
| (1,890)  | 1:41:A:VAL:H     | 1:42:A:ALA:HB3   | 8        | 0.52          |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 8        | 0.52          |
| (1,826)  | 1:35:A:LYS:H     | 1:35:A:LYS:HD3   | 6        | 0.52          |
| (1,826)  | 1:35:A:LYS:H     | 1:35:A:LYS:HD3   | 10       | 0.52          |
| (1,745)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HD22 | 9        | 0.52          |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 2        | 0.52          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 8        | 0.52          |
| (1,468)  | 1:44:A:GLU:HG3   | 1:40:A:ILE:HG21  | 2        | 0.52          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG11  | 3        | 0.52          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG13  | 7        | 0.52          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG11  | 9        | 0.52          |
| (1,358)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HB3  | 6        | 0.52          |
| (1,132)  | 1:41:A:VAL:HG21  | 1:45:A:SER:HB2   | 2        | 0.52          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB3   | 7        | 0.52          |
| (1,1523) | 1:140:A:SER:HB2  | 1:139:A:GLY:H    | 8        | 0.51          |
| (1,1491) | 1:43:A:LEU:HD11  | 1:39:A:ASP:HA    | 2        | 0.51          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 7        | 0.51          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 10       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1340) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD22 | 9        | 0.51          |
| (1,1340) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD22 | 10       | 0.51          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG23  | 3        | 0.51          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD11 | 5        | 0.51          |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD13  | 7        | 0.51          |
| (1,1282) | 1:98:A:TYR:H     | 1:99:A:GLN:HE21  | 9        | 0.51          |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 5        | 0.51          |
| (1,1262) | 1:134:A:SER:H    | 1:132:A:GLY:HA3  | 7        | 0.51          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD11  | 7        | 0.51          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG23 | 2        | 0.51          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 2        | 0.51          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 5        | 0.51          |
| (1,1147) | 1:101:A:VAL:HG21 | 1:105:A:ARG:H    | 1        | 0.51          |
| (1,1147) | 1:101:A:VAL:HG23 | 1:105:A:ARG:H    | 9        | 0.51          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD13  | 2        | 0.51          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 2        | 0.51          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 3        | 0.51          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 7        | 0.51          |
| (1,831)  | 1:119:A:MET:H    | 1:119:A:MET:HB3  | 4        | 0.51          |
| (1,766)  | 1:131:A:VAL:HG21 | 1:128:A:ASN:HB3  | 4        | 0.51          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 2        | 0.51          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 4        | 0.51          |
| (1,642)  | 1:46:A:ALA:HB2   | 1:85:A:TYR:HD1   | 2        | 0.51          |
| (1,556)  | 1:93:A:PRO:HB3   | 1:32:A:ASP:HA    | 10       | 0.51          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 6        | 0.51          |
| (1,451)  | 1:109:A:VAL:HG13 | 1:100:A:LEU:HD11 | 2        | 0.51          |
| (1,358)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HB3  | 1        | 0.51          |
| (1,275)  | 1:119:A:MET:HB3  | 1:122:A:THR:HG21 | 9        | 0.51          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 9        | 0.51          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD2   | 9        | 0.51          |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD2   | 1        | 0.5           |
| (1,1523) | 1:140:A:SER:HB2  | 1:139:A:GLY:H    | 3        | 0.5           |
| (1,1523) | 1:140:A:SER:HB3  | 1:139:A:GLY:H    | 4        | 0.5           |
| (1,1506) | 1:66:A:ALA:HB3   | 1:71:A:PRO:HB2   | 2        | 0.5           |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 2        | 0.5           |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 7        | 0.5           |
| (1,1340) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD22 | 3        | 0.5           |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG23  | 8        | 0.5           |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG21  | 9        | 0.5           |
| (1,1291) | 1:45:A:SER:H     | 1:47:A:LEU:HD11  | 1        | 0.5           |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 1        | 0.5           |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG21 | 9        | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1176) | 1:26:A:GLY:H     | 1:24:A:GLY:HA3   | 9        | 0.5           |
| (1,1171) | 1:100:A:LEU:HD22 | 1:101:A:VAL:H    | 5        | 0.5           |
| (1,1147) | 1:101:A:VAL:HG23 | 1:105:A:ARG:H    | 8        | 0.5           |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 2        | 0.5           |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 6        | 0.5           |
| (1,720)  | 1:108:A:LYS:HA   | 1:103:A:PRO:HB2  | 6        | 0.5           |
| (1,632)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HG2   | 5        | 0.5           |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 7        | 0.5           |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG13  | 4        | 0.5           |
| (1,358)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HB3  | 4        | 0.5           |
| (1,335)  | 1:52:A:LEU:HD21  | 1:49:A:MET:HG2   | 5        | 0.5           |
| (1,132)  | 1:41:A:VAL:HG23  | 1:45:A:SER:HB2   | 1        | 0.5           |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 7        | 0.49          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 6        | 0.49          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG23  | 1        | 0.49          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD12 | 3        | 0.49          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 7        | 0.49          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 8        | 0.49          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB1   | 2        | 0.49          |
| (1,1261) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD21 | 6        | 0.49          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG23 | 4        | 0.49          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB2   | 2        | 0.49          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB2   | 9        | 0.49          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB3   | 9        | 0.49          |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB3   | 10       | 0.49          |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD2   | 10       | 0.49          |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD2   | 3        | 0.49          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 9        | 0.49          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 3        | 0.49          |
| (1,1014) | 1:109:A:VAL:HG13 | 1:110:A:ASP:H    | 1        | 0.49          |
| (1,1014) | 1:109:A:VAL:HG11 | 1:110:A:ASP:H    | 10       | 0.49          |
| (1,766)  | 1:131:A:VAL:HG21 | 1:128:A:ASN:HB3  | 9        | 0.49          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB3  | 4        | 0.49          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 8        | 0.49          |
| (1,655)  | 1:56:A:ARG:HB3   | 1:57:A:TYR:H     | 1        | 0.49          |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 5        | 0.49          |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 9        | 0.49          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG11  | 8        | 0.49          |
| (1,132)  | 1:41:A:VAL:HG22  | 1:45:A:SER:HB2   | 9        | 0.49          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 10       | 0.49          |
| (1,87)   | 1:37:A:ILE:HD13  | 1:126:A:ILE:HA   | 10       | 0.49          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB2   | 10       | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD2   | 7        | 0.48          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 8        | 0.48          |
| (1,1523) | 1:140:A:SER:HB2  | 1:139:A:GLY:H    | 9        | 0.48          |
| (1,1506) | 1:66:A:ALA:HB3   | 1:71:A:PRO:HB2   | 6        | 0.48          |
| (1,1504) | 1:96:A:ALA:HB3   | 1:95:A:GLY:H     | 8        | 0.48          |
| (1,1446) | 1:31:A:ALA:HB2   | 1:30:A:LYS:HB3   | 1        | 0.48          |
| (1,1445) | 1:128:A:ASN:HA   | 1:133:A:THR:H    | 4        | 0.48          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 9        | 0.48          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 5        | 0.48          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG21  | 7        | 0.48          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 2        | 0.48          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB3   | 3        | 0.48          |
| (1,1261) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD21 | 4        | 0.48          |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 1        | 0.48          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 4        | 0.48          |
| (1,766)  | 1:131:A:VAL:HG21 | 1:128:A:ASN:HB3  | 5        | 0.48          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 7        | 0.48          |
| (1,525)  | 1:61:A:GLU:HG3   | 1:73:A:THR:HG23  | 9        | 0.48          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG11  | 1        | 0.48          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG11  | 2        | 0.48          |
| (1,358)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HB3  | 8        | 0.48          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 1        | 0.48          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 6        | 0.48          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 10       | 0.48          |
| (1,286)  | 1:132:A:GLY:HA2  | 1:133:A:THR:HG21 | 1        | 0.48          |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 10       | 0.48          |
| (1,134)  | 1:122:A:THR:HG21 | 1:123:A:ASP:H    | 10       | 0.48          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 2        | 0.48          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 3        | 0.48          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 5        | 0.48          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 6        | 0.48          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 9        | 0.48          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB1   | 2        | 0.48          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD11  | 7        | 0.47          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 6        | 0.47          |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD1   | 9        | 0.47          |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD2   | 10       | 0.47          |
| (1,1522) | 1:105:A:ARG:HD2  | 1:106:A:HIS:HA   | 10       | 0.47          |
| (1,1506) | 1:66:A:ALA:HB1   | 1:71:A:PRO:HB2   | 5        | 0.47          |
| (1,1498) | 1:57:A:TYR:HE2   | 1:47:A:LEU:HG    | 10       | 0.47          |
| (1,1473) | 1:78:A:ARG:HD2   | 1:78:A:ARG:H     | 8        | 0.47          |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 6        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1340) | 1:109:A:VAL:HG11 | 1:128:A:ASN:HD22 | 2        | 0.47          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 4        | 0.47          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD11 | 6        | 0.47          |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 9        | 0.47          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 7        | 0.47          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB1   | 7        | 0.47          |
| (1,1176) | 1:26:A:GLY:H     | 1:24:A:GLY:HA3   | 6        | 0.47          |
| (1,1147) | 1:101:A:VAL:HG23 | 1:105:A:ARG:H    | 7        | 0.47          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG22 | 10       | 0.47          |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG2   | 2        | 0.47          |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG3   | 8        | 0.47          |
| (1,803)  | 1:46:A:ALA:HB3   | 1:67:A:LEU:HA    | 3        | 0.47          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 9        | 0.47          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 9        | 0.47          |
| (1,449)  | 1:109:A:VAL:HG12 | 1:108:A:LYS:HD3  | 1        | 0.47          |
| (1,431)  | 1:40:A:ILE:HB    | 1:41:A:VAL:HG13  | 10       | 0.47          |
| (1,360)  | 1:64:A:LEU:HD12  | 1:68:A:VAL:H     | 7        | 0.47          |
| (1,359)  | 1:64:A:LEU:HD12  | 1:67:A:LEU:H     | 10       | 0.47          |
| (1,335)  | 1:52:A:LEU:HD22  | 1:49:A:MET:HG2   | 1        | 0.47          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 10       | 0.47          |
| (1,189)  | 1:121:A:ASP:HA   | 1:121:A:ASP:HB2  | 3        | 0.47          |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB3   | 9        | 0.47          |
| (1,132)  | 1:41:A:VAL:HG23  | 1:45:A:SER:HB2   | 8        | 0.47          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 1        | 0.47          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 4        | 0.47          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 7        | 0.47          |
| (1,105)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HG12  | 8        | 0.47          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB2   | 5        | 0.47          |
| (1,4)    | 1:126:A:ILE:HG23 | 1:126:A:ILE:H    | 10       | 0.47          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 1        | 0.46          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 10       | 0.46          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 1        | 0.46          |
| (1,1498) | 1:57:A:TYR:HE1   | 1:47:A:LEU:HG    | 1        | 0.46          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 7        | 0.46          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 4        | 0.46          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 8        | 0.46          |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE2   | 2        | 0.46          |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG13 | 8        | 0.46          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB1   | 3        | 0.46          |
| (1,1238) | 1:34:A:GLN:H     | 1:31:A:ALA:HB1   | 8        | 0.46          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB2   | 6        | 0.46          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 4        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1171) | 1:100:A:LEU:HD21 | 1:101:A:VAL:H    | 6        | 0.46          |
| (1,1147) | 1:101:A:VAL:HG22 | 1:105:A:ARG:H    | 2        | 0.46          |
| (1,1014) | 1:109:A:VAL:HG13 | 1:110:A:ASP:H    | 7        | 0.46          |
| (1,806)  | 1:37:A:ILE:HG21  | 1:34:A:GLN:HE22  | 5        | 0.46          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB2  | 9        | 0.46          |
| (1,667)  | 1:109:A:VAL:HG22 | 1:108:A:LYS:HB2  | 9        | 0.46          |
| (1,642)  | 1:46:A:ALA:HB3   | 1:85:A:TYR:HD1   | 3        | 0.46          |
| (1,642)  | 1:46:A:ALA:HB1   | 1:85:A:TYR:HD2   | 6        | 0.46          |
| (1,451)  | 1:109:A:VAL:HG11 | 1:100:A:LEU:HD11 | 7        | 0.46          |
| (1,421)  | 1:129:A:TRP:HB2  | 1:106:A:HIS:HB2  | 2        | 0.46          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 1        | 0.46          |
| (1,335)  | 1:52:A:LEU:HD23  | 1:49:A:MET:HG2   | 8        | 0.46          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 5        | 0.46          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB3   | 3        | 0.46          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB3   | 4        | 0.46          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 1        | 0.45          |
| (1,1575) | 1:118:A:GLY:H    | 1:114:A:TYR:HD2  | 10       | 0.45          |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG21  | 2        | 0.45          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 1        | 0.45          |
| (1,1503) | 1:126:A:ILE:HB   | 1:113:A:SER:HA   | 5        | 0.45          |
| (1,1498) | 1:57:A:TYR:HE1   | 1:47:A:LEU:HG    | 4        | 0.45          |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 8        | 0.45          |
| (1,1446) | 1:31:A:ALA:HB1   | 1:30:A:LYS:HB3   | 9        | 0.45          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 5        | 0.45          |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 4        | 0.45          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG21  | 5        | 0.45          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 10       | 0.45          |
| (1,1292) | 1:34:A:GLN:HE22  | 1:30:A:LYS:HE3   | 3        | 0.45          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB3   | 9        | 0.45          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD13  | 2        | 0.45          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 9        | 0.45          |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB2   | 4        | 0.45          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD12  | 3        | 0.45          |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD2   | 2        | 0.45          |
| (1,1014) | 1:109:A:VAL:HG11 | 1:110:A:ASP:H    | 6        | 0.45          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 10       | 0.45          |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 4        | 0.45          |
| (1,736)  | 1:86:A:ILE:HG23  | 1:85:A:TYR:HD1   | 9        | 0.45          |
| (1,676)  | 1:109:A:VAL:HG22 | 1:100:A:LEU:HA   | 5        | 0.45          |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD23  | 7        | 0.45          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 6        | 0.45          |
| (1,451)  | 1:109:A:VAL:HG12 | 1:100:A:LEU:HD12 | 6        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,354)  | 1:140:A:SER:HB2  | 1:141:A:ASN:H    | 1        | 0.45          |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB2  | 5        | 0.45          |
| (1,335)  | 1:52:A:LEU:HD21  | 1:49:A:MET:HG2   | 3        | 0.45          |
| (1,196)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HB2   | 2        | 0.45          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD12  | 9        | 0.45          |
| (1,4)    | 1:126:A:ILE:HG21 | 1:126:A:ILE:H    | 1        | 0.45          |
| (1,4)    | 1:126:A:ILE:HG22 | 1:126:A:ILE:H    | 5        | 0.45          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 2        | 0.44          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 5        | 0.44          |
| (1,1444) | 1:27:A:ASN:HB3   | 1:28:A:LYS:HB2   | 4        | 0.44          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 2        | 0.44          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG23  | 4        | 0.44          |
| (1,1306) | 1:109:A:VAL:H    | 1:100:A:LEU:HD13 | 1        | 0.44          |
| (1,1290) | 1:38:A:SER:H     | 1:36:A:ALA:HB2   | 6        | 0.44          |
| (1,1261) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD21 | 5        | 0.44          |
| (1,1245) | 1:40:A:ILE:HD11  | 1:37:A:ILE:H     | 4        | 0.44          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB3   | 4        | 0.44          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG22 | 4        | 0.44          |
| (1,1171) | 1:100:A:LEU:HD23 | 1:101:A:VAL:H    | 2        | 0.44          |
| (1,1171) | 1:100:A:LEU:HD23 | 1:101:A:VAL:H    | 3        | 0.44          |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB1   | 3        | 0.44          |
| (1,1014) | 1:109:A:VAL:HG13 | 1:110:A:ASP:H    | 5        | 0.44          |
| (1,953)  | 1:65:A:GLY:HA3   | 1:67:A:LEU:H     | 5        | 0.44          |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2   | 9        | 0.44          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 7        | 0.44          |
| (1,738)  | 1:78:A:ARG:HD2   | 1:54:A:ASN:H     | 1        | 0.44          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB2  | 10       | 0.44          |
| (1,676)  | 1:109:A:VAL:HG21 | 1:100:A:LEU:HA   | 4        | 0.44          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 6        | 0.44          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 7        | 0.44          |
| (1,525)  | 1:61:A:GLU:HG3   | 1:73:A:THR:HG23  | 3        | 0.44          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 8        | 0.44          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB3   | 6        | 0.44          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 7        | 0.44          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG21 | 9        | 0.44          |
| (1,360)  | 1:64:A:LEU:HD11  | 1:68:A:VAL:H     | 2        | 0.44          |
| (1,358)  | 1:64:A:LEU:HD22  | 1:100:A:LEU:HB3  | 5        | 0.44          |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB3  | 2        | 0.44          |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB3  | 9        | 0.44          |
| (1,334)  | 1:52:A:LEU:HD22  | 1:51:A:LYS:HG2   | 6        | 0.44          |
| (1,132)  | 1:41:A:VAL:HG23  | 1:45:A:SER:HB2   | 5        | 0.44          |
| (1,132)  | 1:41:A:VAL:HG22  | 1:45:A:SER:HB2   | 6        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,132)  | 1:41:A:VAL:HG21  | 1:45:A:SER:HB2   | 10       | 0.44          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB2   | 8        | 0.44          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD12  | 5        | 0.44          |
| (1,4)    | 1:126:A:ILE:HG23 | 1:126:A:ILE:H    | 4        | 0.44          |
| (1,4)    | 1:126:A:ILE:HG21 | 1:126:A:ILE:H    | 7        | 0.44          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 3        | 0.43          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 6        | 0.43          |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD1   | 5        | 0.43          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 7        | 0.43          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 9        | 0.43          |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 10       | 0.43          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 4        | 0.43          |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD1   | 1        | 0.43          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG21  | 6        | 0.43          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB2   | 10       | 0.43          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 2        | 0.43          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 9        | 0.43          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 10       | 0.43          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 10       | 0.43          |
| (1,1171) | 1:100:A:LEU:HD21 | 1:101:A:VAL:H    | 1        | 0.43          |
| (1,1171) | 1:100:A:LEU:HD22 | 1:101:A:VAL:H    | 7        | 0.43          |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB2   | 2        | 0.43          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD13  | 4        | 0.43          |
| (1,1006) | 1:108:A:LYS:HB2  | 1:109:A:VAL:H    | 4        | 0.43          |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG3   | 7        | 0.43          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA3  | 10       | 0.43          |
| (1,803)  | 1:46:A:ALA:HB2   | 1:67:A:LEU:HA    | 4        | 0.43          |
| (1,738)  | 1:78:A:ARG:HD2   | 1:54:A:ASN:H     | 2        | 0.43          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB2  | 1        | 0.43          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 1        | 0.43          |
| (1,719)  | 1:45:A:SER:HB2   | 1:48:A:ASP:HB2   | 6        | 0.43          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 4        | 0.43          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 8        | 0.43          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 10       | 0.43          |
| (1,451)  | 1:109:A:VAL:HG12 | 1:100:A:LEU:HD11 | 10       | 0.43          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG21 | 8        | 0.43          |
| (1,360)  | 1:64:A:LEU:HD12  | 1:68:A:VAL:H     | 4        | 0.43          |
| (1,304)  | 1:72:A:THR:HG22  | 1:73:A:THR:H     | 6        | 0.43          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 3        | 0.43          |
| (1,52)   | 1:33:A:ARG:HD2   | 1:37:A:ILE:HD13  | 6        | 0.43          |
| (1,4)    | 1:126:A:ILE:HG21 | 1:126:A:ILE:H    | 6        | 0.43          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 3        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 4        | 0.42          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 6        | 0.42          |
| (1,1529) | 1:59:A:THR:H     | 1:62:A:GLN:HA    | 10       | 0.42          |
| (1,1498) | 1:57:A:TYR:HE1   | 1:47:A:LEU:HG    | 9        | 0.42          |
| (1,1462) | 1:45:A:SER:HB2   | 1:44:A:GLU:HB3   | 8        | 0.42          |
| (1,1319) | 1:42:A:ALA:H     | 1:40:A:ILE:HG22  | 2        | 0.42          |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE3   | 9        | 0.42          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD11  | 9        | 0.42          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB2   | 1        | 0.42          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG21 | 1        | 0.42          |
| (1,1171) | 1:100:A:LEU:HD23 | 1:101:A:VAL:H    | 8        | 0.42          |
| (1,806)  | 1:37:A:ILE:HG22  | 1:34:A:GLN:HE22  | 6        | 0.42          |
| (1,806)  | 1:37:A:ILE:HG23  | 1:34:A:GLN:HE22  | 9        | 0.42          |
| (1,803)  | 1:46:A:ALA:HB2   | 1:67:A:LEU:HA    | 2        | 0.42          |
| (1,633)  | 1:79:A:SER:HB3   | 1:79:A:SER:H     | 7        | 0.42          |
| (1,616)  | 1:100:A:LEU:HD21 | 1:58:A:PRO:HG2   | 5        | 0.42          |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 3        | 0.42          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 4        | 0.42          |
| (1,379)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:HA3  | 10       | 0.42          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG23 | 2        | 0.42          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG23 | 6        | 0.42          |
| (1,360)  | 1:64:A:LEU:HD11  | 1:68:A:VAL:H     | 6        | 0.42          |
| (1,335)  | 1:52:A:LEU:HD21  | 1:49:A:MET:HG2   | 2        | 0.42          |
| (1,199)  | 1:111:A:VAL:HG12 | 1:112:A:PHE:H    | 1        | 0.42          |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 5        | 0.42          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 6        | 0.42          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 7        | 0.42          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 10       | 0.42          |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 6        | 0.42          |
| (1,134)  | 1:122:A:THR:HG23 | 1:123:A:ASP:H    | 9        | 0.42          |
| (1,1537) | 1:50:A:TYR:H     | 1:50:A:TYR:HD1   | 8        | 0.41          |
| (1,1506) | 1:66:A:ALA:HB3   | 1:71:A:PRO:HB2   | 4        | 0.41          |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 5        | 0.41          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 2        | 0.41          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB2   | 7        | 0.41          |
| (1,1176) | 1:26:A:GLY:H     | 1:24:A:GLY:HA3   | 4        | 0.41          |
| (1,1176) | 1:26:A:GLY:H     | 1:24:A:GLY:HA3   | 5        | 0.41          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 4        | 0.41          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 7        | 0.41          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 4        | 0.41          |
| (1,978)  | 1:98:A:TYR:HB3   | 1:98:A:TYR:H     | 1        | 0.41          |
| (1,803)  | 1:46:A:ALA:HB1   | 1:67:A:LEU:HA    | 6        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,779)  | 1:40:A:ILE:HG21  | 1:112:A:PHE:HA   | 3        | 0.41          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB2  | 2        | 0.41          |
| (1,664)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HA   | 4        | 0.41          |
| (1,659)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HA    | 3        | 0.41          |
| (1,633)  | 1:79:A:SER:HB3   | 1:79:A:SER:H     | 2        | 0.41          |
| (1,633)  | 1:79:A:SER:HB3   | 1:79:A:SER:H     | 3        | 0.41          |
| (1,556)  | 1:93:A:PRO:HB3   | 1:32:A:ASP:HA    | 1        | 0.41          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 3        | 0.41          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 2        | 0.41          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB3   | 7        | 0.41          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG22 | 1        | 0.41          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG21 | 7        | 0.41          |
| (1,360)  | 1:64:A:LEU:HD12  | 1:68:A:VAL:H     | 8        | 0.41          |
| (1,335)  | 1:52:A:LEU:HD21  | 1:49:A:MET:HG2   | 6        | 0.41          |
| (1,304)  | 1:72:A:THR:HG22  | 1:73:A:THR:H     | 4        | 0.41          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG12 | 1        | 0.41          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 9        | 0.41          |
| (1,134)  | 1:122:A:THR:HG21 | 1:123:A:ASP:H    | 6        | 0.41          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB2   | 1        | 0.41          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 4        | 0.41          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 6        | 0.4           |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 7        | 0.4           |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 7        | 0.4           |
| (1,1523) | 1:140:A:SER:HB2  | 1:139:A:GLY:H    | 2        | 0.4           |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 2        | 0.4           |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 2        | 0.4           |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD12  | 6        | 0.4           |
| (1,1245) | 1:40:A:ILE:HD13  | 1:37:A:ILE:H     | 10       | 0.4           |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB1   | 7        | 0.4           |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB2   | 8        | 0.4           |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 9        | 0.4           |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD11  | 1        | 0.4           |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD13  | 5        | 0.4           |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 1        | 0.4           |
| (1,1062) | 1:100:A:LEU:HD21 | 1:64:A:LEU:H     | 4        | 0.4           |
| (1,1062) | 1:100:A:LEU:HD23 | 1:64:A:LEU:H     | 5        | 0.4           |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG2   | 5        | 0.4           |
| (1,664)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HA   | 6        | 0.4           |
| (1,664)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HA   | 7        | 0.4           |
| (1,616)  | 1:100:A:LEU:HD22 | 1:58:A:PRO:HG2   | 4        | 0.4           |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD23  | 4        | 0.4           |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 8        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 2        | 0.4           |
| (1,556)  | 1:93:A:PRO:HB3   | 1:32:A:ASP:HA    | 4        | 0.4           |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 7        | 0.4           |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 8        | 0.4           |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB3   | 10       | 0.4           |
| (1,484)  | 1:59:A:THR:HG22  | 1:62:A:GLN:HG2   | 9        | 0.4           |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 2        | 0.4           |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 8        | 0.4           |
| (1,451)  | 1:109:A:VAL:HG11 | 1:100:A:LEU:HD11 | 1        | 0.4           |
| (1,335)  | 1:52:A:LEU:HD22  | 1:49:A:MET:HG2   | 9        | 0.4           |
| (1,334)  | 1:52:A:LEU:HD22  | 1:51:A:LYS:HG2   | 2        | 0.4           |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 5        | 0.4           |
| (1,304)  | 1:72:A:THR:HG21  | 1:73:A:THR:H     | 10       | 0.4           |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 9        | 0.4           |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 2        | 0.4           |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG11 | 3        | 0.4           |
| (1,134)  | 1:122:A:THR:HG23 | 1:123:A:ASP:H    | 7        | 0.4           |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 5        | 0.4           |
| (1,4)    | 1:126:A:ILE:HG21 | 1:126:A:ILE:H    | 8        | 0.4           |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 2        | 0.39          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD13  | 9        | 0.39          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 10       | 0.39          |
| (1,1462) | 1:45:A:SER:HB2   | 1:44:A:GLU:HB3   | 4        | 0.39          |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE2   | 2        | 0.39          |
| (1,1262) | 1:134:A:SER:H    | 1:132:A:GLY:HA2  | 8        | 0.39          |
| (1,1261) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD21 | 10       | 0.39          |
| (1,1245) | 1:40:A:ILE:HD13  | 1:37:A:ILE:H     | 3        | 0.39          |
| (1,1245) | 1:40:A:ILE:HD13  | 1:37:A:ILE:H     | 8        | 0.39          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB3   | 2        | 0.39          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB1   | 3        | 0.39          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 8        | 0.39          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 2        | 0.39          |
| (1,1062) | 1:100:A:LEU:HD21 | 1:64:A:LEU:H     | 3        | 0.39          |
| (1,1062) | 1:100:A:LEU:HD21 | 1:64:A:LEU:H     | 8        | 0.39          |
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 8        | 0.39          |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG3   | 9        | 0.39          |
| (1,806)  | 1:37:A:ILE:HG23  | 1:34:A:GLN:HE22  | 10       | 0.39          |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD21  | 3        | 0.39          |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD21  | 6        | 0.39          |
| (1,664)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HA   | 5        | 0.39          |
| (1,618)  | 1:100:A:LEU:HD23 | 1:100:A:LEU:H    | 7        | 0.39          |
| (1,616)  | 1:100:A:LEU:HD22 | 1:58:A:PRO:HG2   | 2        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD21  | 10       | 0.39          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 1        | 0.39          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 3        | 0.39          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 9        | 0.39          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG21  | 10       | 0.39          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 9        | 0.39          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 5        | 0.39          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 1        | 0.39          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB3   | 2        | 0.39          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB2   | 3        | 0.39          |
| (1,484)  | 1:59:A:THR:HG23  | 1:62:A:GLN:HG2   | 1        | 0.39          |
| (1,484)  | 1:59:A:THR:HG23  | 1:62:A:GLN:HG2   | 5        | 0.39          |
| (1,360)  | 1:64:A:LEU:HD12  | 1:68:A:VAL:H     | 3        | 0.39          |
| (1,258)  | 1:76:A:GLU:HB2   | 1:72:A:THR:HA    | 10       | 0.39          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 2        | 0.39          |
| (1,228)  | 1:63:A:GLY:HA2   | 1:100:A:LEU:HB2  | 1        | 0.39          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB1   | 7        | 0.39          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD11  | 2        | 0.39          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 9        | 0.38          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 5        | 0.38          |
| (1,1506) | 1:66:A:ALA:HB2   | 1:71:A:PRO:HB2   | 9        | 0.38          |
| (1,1503) | 1:126:A:ILE:HB   | 1:113:A:SER:HA   | 7        | 0.38          |
| (1,1470) | 1:86:A:ILE:HG21  | 1:85:A:TYR:H     | 3        | 0.38          |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2   | 10       | 0.38          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 3        | 0.38          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 6        | 0.38          |
| (1,1268) | 1:70:A:LYS:H     | 1:69:A:LYS:HE2   | 3        | 0.38          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD13  | 3        | 0.38          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 5        | 0.38          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB1   | 8        | 0.38          |
| (1,1163) | 1:79:A:SER:H     | 1:78:A:ARG:HB2   | 3        | 0.38          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG2   | 5        | 0.38          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG2   | 7        | 0.38          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD12  | 7        | 0.38          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 7        | 0.38          |
| (1,1062) | 1:100:A:LEU:HD22 | 1:64:A:LEU:H     | 6        | 0.38          |
| (1,1062) | 1:100:A:LEU:HD23 | 1:64:A:LEU:H     | 7        | 0.38          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG23 | 3        | 0.38          |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG2   | 6        | 0.38          |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 8        | 0.38          |
| (1,810)  | 1:36:A:ALA:HA    | 1:113:A:SER:HB2  | 1        | 0.38          |
| (1,810)  | 1:36:A:ALA:HA    | 1:113:A:SER:HB2  | 10       | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD21  | 5        | 0.38          |
| (1,728)  | 1:88:A:ARG:HD2   | 1:89:A:LEU:HA    | 5        | 0.38          |
| (1,664)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HA   | 1        | 0.38          |
| (1,650)  | 1:32:A:ASP:HB2   | 1:93:A:PRO:HB2   | 2        | 0.38          |
| (1,618)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:H    | 2        | 0.38          |
| (1,618)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:H    | 6        | 0.38          |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD22  | 8        | 0.38          |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 2        | 0.38          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 10       | 0.38          |
| (1,556)  | 1:93:A:PRO:HB2   | 1:32:A:ASP:HA    | 6        | 0.38          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 10       | 0.38          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB1   | 1        | 0.38          |
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG22  | 8        | 0.38          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 6        | 0.38          |
| (1,423)  | 1:49:A:MET:HG3   | 1:49:A:MET:HA    | 10       | 0.38          |
| (1,335)  | 1:52:A:LEU:HD21  | 1:49:A:MET:HG2   | 4        | 0.38          |
| (1,334)  | 1:52:A:LEU:HD23  | 1:51:A:LYS:HG2   | 1        | 0.38          |
| (1,334)  | 1:52:A:LEU:HD22  | 1:51:A:LYS:HG2   | 3        | 0.38          |
| (1,258)  | 1:76:A:GLU:HB3   | 1:72:A:THR:HA    | 4        | 0.38          |
| (1,258)  | 1:76:A:GLU:HB2   | 1:72:A:THR:HA    | 8        | 0.38          |
| (1,220)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HD2  | 2        | 0.38          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 8        | 0.38          |
| (1,134)  | 1:122:A:THR:HG22 | 1:123:A:ASP:H    | 8        | 0.38          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB2   | 6        | 0.38          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 6        | 0.38          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD12  | 1        | 0.38          |
| (1,1474) | 1:56:A:ARG:HD2   | 1:50:A:TYR:HE1   | 7        | 0.37          |
| (1,1474) | 1:56:A:ARG:HD3   | 1:50:A:TYR:HE2   | 8        | 0.37          |
| (1,1472) | 1:78:A:ARG:HD3   | 1:78:A:ARG:HB2   | 2        | 0.37          |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 4        | 0.37          |
| (1,1446) | 1:31:A:ALA:HB3   | 1:30:A:LYS:HB3   | 6        | 0.37          |
| (1,1444) | 1:27:A:ASN:HB3   | 1:30:A:LYS:HB3   | 1        | 0.37          |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE1   | 5        | 0.37          |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2   | 8        | 0.37          |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 7        | 0.37          |
| (1,1245) | 1:40:A:ILE:HD13  | 1:37:A:ILE:H     | 1        | 0.37          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB2   | 8        | 0.37          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 1        | 0.37          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 6        | 0.37          |
| (1,1176) | 1:26:A:GLY:H     | 1:24:A:GLY:HA2   | 1        | 0.37          |
| (1,1171) | 1:100:A:LEU:HD23 | 1:101:A:VAL:H    | 9        | 0.37          |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 5        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG2   | 6        | 0.37          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD11  | 9        | 0.37          |
| (1,1118) | 1:89:A:LEU:H     | 1:86:A:ILE:HD11  | 10       | 0.37          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 8        | 0.37          |
| (1,1062) | 1:100:A:LEU:HD23 | 1:64:A:LEU:H     | 10       | 0.37          |
| (1,779)  | 1:40:A:ILE:HG22  | 1:112:A:PHE:HA   | 7        | 0.37          |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD23  | 8        | 0.37          |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 4        | 0.37          |
| (1,699)  | 1:101:A:VAL:HG22 | 1:105:A:ARG:HD2  | 2        | 0.37          |
| (1,676)  | 1:109:A:VAL:HG21 | 1:100:A:LEU:HA   | 6        | 0.37          |
| (1,657)  | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD12  | 3        | 0.37          |
| (1,655)  | 1:56:A:ARG:HB3   | 1:57:A:TYR:H     | 10       | 0.37          |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD23  | 6        | 0.37          |
| (1,587)  | 1:48:A:ASP:HB2   | 1:49:A:MET:H     | 5        | 0.37          |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 10       | 0.37          |
| (1,578)  | 1:86:A:ILE:HG12  | 1:87:A:ARG:H     | 5        | 0.37          |
| (1,544)  | 1:57:A:TYR:HA    | 1:57:A:TYR:HD1   | 5        | 0.37          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB3   | 4        | 0.37          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB1   | 5        | 0.37          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB2   | 8        | 0.37          |
| (1,484)  | 1:59:A:THR:HG21  | 1:62:A:GLN:HG2   | 3        | 0.37          |
| (1,358)  | 1:64:A:LEU:HD21  | 1:100:A:LEU:HB3  | 3        | 0.37          |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB3  | 1        | 0.37          |
| (1,334)  | 1:52:A:LEU:HD23  | 1:51:A:LYS:HG2   | 9        | 0.37          |
| (1,258)  | 1:76:A:GLU:HB3   | 1:72:A:THR:HA    | 2        | 0.37          |
| (1,258)  | 1:76:A:GLU:HB2   | 1:72:A:THR:HA    | 3        | 0.37          |
| (1,258)  | 1:76:A:GLU:HB3   | 1:72:A:THR:HA    | 6        | 0.37          |
| (1,253)  | 1:92:A:ASP:HB2   | 1:113:A:SER:HB3  | 1        | 0.37          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 5        | 0.37          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 10       | 0.37          |
| (1,183)  | 1:32:A:ASP:HB3   | 1:28:A:LYS:HG3   | 3        | 0.37          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 4        | 0.37          |
| (1,176)  | 1:100:A:LEU:HB3  | 1:111:A:VAL:HG13 | 5        | 0.37          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 6        | 0.37          |
| (1,52)   | 1:33:A:ARG:HD2   | 1:37:A:ILE:HD11  | 1        | 0.37          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB3   | 8        | 0.37          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD13  | 3        | 0.37          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD12  | 10       | 0.37          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 4        | 0.36          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 9        | 0.36          |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB1   | 6        | 0.36          |
| (1,1580) | 1:48:A:ASP:H     | 1:52:A:LEU:HD13  | 10       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1543) | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 9        | 0.36          |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 2        | 0.36          |
| (1,1462) | 1:45:A:SER:HB2   | 1:44:A:GLU:HB3   | 9        | 0.36          |
| (1,1439) | 1:79:A:SER:H     | 1:78:A:ARG:HD3   | 8        | 0.36          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 7        | 0.36          |
| (1,1340) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD22 | 7        | 0.36          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD2   | 8        | 0.36          |
| (1,1261) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD21 | 3        | 0.36          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG21 | 7        | 0.36          |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB3   | 6        | 0.36          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG2   | 9        | 0.36          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG3   | 10       | 0.36          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 2        | 0.36          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 6        | 0.36          |
| (1,1014) | 1:109:A:VAL:HG11 | 1:110:A:ASP:H    | 4        | 0.36          |
| (1,803)  | 1:46:A:ALA:HB3   | 1:67:A:LEU:HA    | 8        | 0.36          |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD2  | 8        | 0.36          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB2  | 8        | 0.36          |
| (1,664)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HA   | 2        | 0.36          |
| (1,664)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HA   | 10       | 0.36          |
| (1,659)  | 1:111:A:VAL:HG21 | 1:40:A:ILE:HA    | 6        | 0.36          |
| (1,618)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:H    | 8        | 0.36          |
| (1,616)  | 1:100:A:LEU:HD21 | 1:58:A:PRO:HG2   | 7        | 0.36          |
| (1,603)  | 1:98:A:TYR:HB3   | 1:64:A:LEU:HD22  | 3        | 0.36          |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 5        | 0.36          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 2        | 0.36          |
| (1,499)  | 1:71:A:PRO:HA    | 1:66:A:ALA:HB2   | 9        | 0.36          |
| (1,336)  | 1:52:A:LEU:HD13  | 1:48:A:ASP:HB3   | 7        | 0.36          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 7        | 0.36          |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 2        | 0.36          |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 7        | 0.36          |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB3   | 3        | 0.36          |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB3   | 8        | 0.36          |
| (1,84)   | 1:37:A:ILE:HA    | 1:36:A:ALA:HB3   | 9        | 0.36          |
| (1,52)   | 1:33:A:ARG:HD2   | 1:37:A:ILE:HD12  | 7        | 0.36          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 8        | 0.35          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 10       | 0.35          |
| (1,1575) | 1:118:A:GLY:H    | 1:114:A:TYR:HD2  | 3        | 0.35          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD11  | 8        | 0.35          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 8        | 0.35          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 7        | 0.35          |
| (1,1503) | 1:89:A:LEU:HB2   | 1:88:A:ARG:HA    | 6        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 9        | 0.35          |
| (1,1470) | 1:86:A:ILE:HG22  | 1:85:A:TYR:H     | 8        | 0.35          |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 1        | 0.35          |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 3        | 0.35          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 10       | 0.35          |
| (1,1368) | 1:32:A:ASP:H     | 1:28:A:LYS:HB3   | 9        | 0.35          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 6        | 0.35          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 9        | 0.35          |
| (1,1262) | 1:134:A:SER:H    | 1:132:A:GLY:HA3  | 1        | 0.35          |
| (1,1245) | 1:40:A:ILE:HD13  | 1:37:A:ILE:H     | 2        | 0.35          |
| (1,1245) | 1:40:A:ILE:HD12  | 1:37:A:ILE:H     | 5        | 0.35          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB3   | 7        | 0.35          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB3   | 4        | 0.35          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG22 | 6        | 0.35          |
| (1,1171) | 1:100:A:LEU:HD22 | 1:101:A:VAL:H    | 10       | 0.35          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG3   | 8        | 0.35          |
| (1,1110) | 1:36:A:ALA:H     | 1:35:A:LYS:HD2   | 7        | 0.35          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 4        | 0.35          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 5        | 0.35          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 3        | 0.35          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 4        | 0.35          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 5        | 0.35          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 6        | 0.35          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 7        | 0.35          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 9        | 0.35          |
| (1,1062) | 1:100:A:LEU:HD21 | 1:64:A:LEU:H     | 9        | 0.35          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG21 | 1        | 0.35          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG21 | 4        | 0.35          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG23 | 5        | 0.35          |
| (1,978)  | 1:98:A:TYR:HB3   | 1:98:A:TYR:H     | 3        | 0.35          |
| (1,978)  | 1:98:A:TYR:HB3   | 1:98:A:TYR:H     | 4        | 0.35          |
| (1,978)  | 1:98:A:TYR:HB3   | 1:98:A:TYR:H     | 6        | 0.35          |
| (1,867)  | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG2   | 4        | 0.35          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 2        | 0.35          |
| (1,738)  | 1:78:A:ARG:HD2   | 1:54:A:ASN:H     | 7        | 0.35          |
| (1,727)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HB2  | 3        | 0.35          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 10       | 0.35          |
| (1,664)  | 1:109:A:VAL:HG23 | 1:109:A:VAL:HA   | 8        | 0.35          |
| (1,633)  | 1:79:A:SER:HB3   | 1:79:A:SER:H     | 5        | 0.35          |
| (1,618)  | 1:100:A:LEU:HD23 | 1:100:A:LEU:H    | 10       | 0.35          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 2        | 0.35          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 1        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 9        | 0.35          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 2        | 0.35          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 4        | 0.35          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 8        | 0.35          |
| (1,201)  | 1:111:A:VAL:HG13 | 1:128:A:ASN:HD21 | 3        | 0.35          |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 4        | 0.35          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 1        | 0.35          |
| (1,1580) | 1:48:A:ASP:H     | 1:67:A:LEU:HD12  | 7        | 0.34          |
| (1,1575) | 1:118:A:GLY:H    | 1:114:A:TYR:HD2  | 6        | 0.34          |
| (1,1503) | 1:89:A:LEU:HB2   | 1:88:A:ARG:HA    | 8        | 0.34          |
| (1,1498) | 1:57:A:TYR:HE1   | 1:47:A:LEU:HG    | 5        | 0.34          |
| (1,1492) | 1:43:A:LEU:HD11  | 1:99:A:GLN:H     | 9        | 0.34          |
| (1,1444) | 1:27:A:ASN:HB3   | 1:30:A:LYS:HB3   | 6        | 0.34          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 1        | 0.34          |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 1        | 0.34          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD13  | 8        | 0.34          |
| (1,1245) | 1:40:A:ILE:HD12  | 1:37:A:ILE:H     | 6        | 0.34          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB1   | 2        | 0.34          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 3        | 0.34          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 10       | 0.34          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 7        | 0.34          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG2   | 1        | 0.34          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 5        | 0.34          |
| (1,1066) | 1:130:A:ASN:HD21 | 1:130:A:ASN:HB2  | 10       | 0.34          |
| (1,1062) | 1:100:A:LEU:HD22 | 1:64:A:LEU:H     | 1        | 0.34          |
| (1,779)  | 1:40:A:ILE:HG23  | 1:112:A:PHE:HA   | 2        | 0.34          |
| (1,779)  | 1:40:A:ILE:HG22  | 1:112:A:PHE:HA   | 6        | 0.34          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 1        | 0.34          |
| (1,676)  | 1:109:A:VAL:HG23 | 1:100:A:LEU:HA   | 1        | 0.34          |
| (1,664)  | 1:109:A:VAL:HG21 | 1:109:A:VAL:HA   | 9        | 0.34          |
| (1,618)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:H    | 9        | 0.34          |
| (1,616)  | 1:100:A:LEU:HD23 | 1:58:A:PRO:HG2   | 1        | 0.34          |
| (1,616)  | 1:100:A:LEU:HD22 | 1:58:A:PRO:HG2   | 3        | 0.34          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 7        | 0.34          |
| (1,544)  | 1:57:A:TYR:HA    | 1:57:A:TYR:HD1   | 9        | 0.34          |
| (1,484)  | 1:59:A:THR:HG22  | 1:62:A:GLN:HG2   | 4        | 0.34          |
| (1,451)  | 1:109:A:VAL:HG11 | 1:100:A:LEU:HD12 | 5        | 0.34          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 3        | 0.34          |
| (1,258)  | 1:76:A:GLU:HB3   | 1:72:A:THR:HA    | 1        | 0.34          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 1        | 0.34          |
| (1,136)  | 1:50:A:TYR:HA    | 1:54:A:ASN:HB3   | 6        | 0.34          |
| (1,134)  | 1:122:A:THR:HG22 | 1:123:A:ASP:H    | 3        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,134)  | 1:122:A:THR:HG23 | 1:123:A:ASP:H    | 4        | 0.34          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 8        | 0.34          |
| (1,95)   | 1:37:A:ILE:HG21  | 1:41:A:VAL:H     | 3        | 0.34          |
| (1,95)   | 1:37:A:ILE:HG23  | 1:41:A:VAL:H     | 5        | 0.34          |
| (1,95)   | 1:37:A:ILE:HG21  | 1:41:A:VAL:H     | 6        | 0.34          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 9        | 0.34          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD11  | 6        | 0.34          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 2        | 0.33          |
| (1,1473) | 1:78:A:ARG:HD2   | 1:78:A:ARG:H     | 6        | 0.33          |
| (1,1472) | 1:78:A:ARG:HD3   | 1:78:A:ARG:HB2   | 4        | 0.33          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG23 | 8        | 0.33          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG23 | 9        | 0.33          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 7        | 0.33          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 6        | 0.33          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB3   | 1        | 0.33          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB1   | 5        | 0.33          |
| (1,1194) | 1:104:A:GLY:H    | 1:109:A:VAL:HG21 | 7        | 0.33          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG2   | 4        | 0.33          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG11 | 3        | 0.33          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 6        | 0.33          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 5        | 0.33          |
| (1,1028) | 1:86:A:ILE:H     | 1:46:A:ALA:HB1   | 7        | 0.33          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG21 | 9        | 0.33          |
| (1,904)  | 1:106:A:HIS:HB3  | 1:107:A:GLY:H    | 4        | 0.33          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 5        | 0.33          |
| (1,803)  | 1:46:A:ALA:HB1   | 1:67:A:LEU:HA    | 7        | 0.33          |
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2   | 4        | 0.33          |
| (1,767)  | 1:122:A:THR:HG22 | 1:121:A:ASP:H    | 1        | 0.33          |
| (1,767)  | 1:122:A:THR:HG21 | 1:121:A:ASP:H    | 3        | 0.33          |
| (1,767)  | 1:122:A:THR:HG21 | 1:121:A:ASP:H    | 8        | 0.33          |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD22  | 1        | 0.33          |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD21  | 4        | 0.33          |
| (1,751)  | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 3        | 0.33          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 5        | 0.33          |
| (1,676)  | 1:109:A:VAL:HG23 | 1:100:A:LEU:HA   | 2        | 0.33          |
| (1,676)  | 1:109:A:VAL:HG23 | 1:100:A:LEU:HA   | 7        | 0.33          |
| (1,667)  | 1:109:A:VAL:HG23 | 1:108:A:LYS:HB2  | 3        | 0.33          |
| (1,657)  | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD11  | 10       | 0.33          |
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB2   | 7        | 0.33          |
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB3   | 10       | 0.33          |
| (1,618)  | 1:100:A:LEU:HD23 | 1:100:A:LEU:H    | 5        | 0.33          |
| (1,616)  | 1:100:A:LEU:HD22 | 1:58:A:PRO:HG2   | 8        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,616)  | 1:100:A:LEU:HD21 | 1:58:A:PRO:HG2   | 10       | 0.33          |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 6        | 0.33          |
| (1,544)  | 1:57:A:TYR:HA    | 1:57:A:TYR:HD2   | 4        | 0.33          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 3        | 0.33          |
| (1,360)  | 1:64:A:LEU:HD11  | 1:68:A:VAL:H     | 5        | 0.33          |
| (1,286)  | 1:132:A:GLY:HA3  | 1:133:A:THR:HG22 | 10       | 0.33          |
| (1,258)  | 1:76:A:GLU:HB2   | 1:72:A:THR:HA    | 5        | 0.33          |
| (1,253)  | 1:92:A:ASP:HB3   | 1:113:A:SER:HB3  | 6        | 0.33          |
| (1,253)  | 1:92:A:ASP:HB2   | 1:113:A:SER:HB3  | 9        | 0.33          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 3        | 0.33          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 6        | 0.33          |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 7        | 0.33          |
| (1,222)  | 1:88:A:ARG:HD2   | 1:88:A:ARG:HB3   | 5        | 0.33          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 10       | 0.33          |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 10       | 0.33          |
| (1,95)   | 1:37:A:ILE:HG23  | 1:41:A:VAL:H     | 1        | 0.33          |
| (1,95)   | 1:37:A:ILE:HG22  | 1:41:A:VAL:H     | 2        | 0.33          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 2        | 0.33          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB1   | 3        | 0.33          |
| (1,1596) | 1:46:A:ALA:H     | 1:47:A:LEU:HB3   | 5        | 0.32          |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB3   | 5        | 0.32          |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB1   | 10       | 0.32          |
| (1,1576) | 1:83:A:ASP:H     | 1:84:A:GLY:HA3   | 8        | 0.32          |
| (1,1569) | 1:92:A:ASP:H     | 1:95:A:GLY:H     | 10       | 0.32          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 5        | 0.32          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 3        | 0.32          |
| (1,1528) | 1:31:A:ALA:HB3   | 1:27:A:ASN:HB3   | 2        | 0.32          |
| (1,1446) | 1:31:A:ALA:HB2   | 1:30:A:LYS:HB3   | 4        | 0.32          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 3        | 0.32          |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2   | 9        | 0.32          |
| (1,1340) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD22 | 1        | 0.32          |
| (1,1282) | 1:98:A:TYR:H     | 1:99:A:GLN:HE21  | 2        | 0.32          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 1        | 0.32          |
| (1,1261) | 1:109:A:VAL:HG11 | 1:128:A:ASN:HD21 | 8        | 0.32          |
| (1,1245) | 1:40:A:ILE:HD11  | 1:37:A:ILE:H     | 7        | 0.32          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB3   | 3        | 0.32          |
| (1,1237) | 1:34:A:GLN:H     | 1:36:A:ALA:HB2   | 5        | 0.32          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 1        | 0.32          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB2   | 10       | 0.32          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG12 | 1        | 0.32          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 2        | 0.32          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 6        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1028) | 1:86:A:ILE:H     | 1:46:A:ALA:HB3   | 3        | 0.32          |
| (1,984)  | 1:96:A:ALA:HB3   | 1:97:A:GLU:H     | 7        | 0.32          |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 4        | 0.32          |
| (1,803)  | 1:46:A:ALA:HB2   | 1:67:A:LEU:HA    | 1        | 0.32          |
| (1,803)  | 1:46:A:ALA:HB1   | 1:67:A:LEU:HA    | 10       | 0.32          |
| (1,772)  | 1:105:A:ARG:HG2  | 1:106:A:HIS:HD2  | 1        | 0.32          |
| (1,767)  | 1:122:A:THR:HG21 | 1:121:A:ASP:H    | 5        | 0.32          |
| (1,758)  | 1:49:A:MET:HG3   | 1:52:A:LEU:HD22  | 9        | 0.32          |
| (1,687)  | 1:98:A:TYR:HB2   | 1:43:A:LEU:HD13  | 1        | 0.32          |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2   | 8        | 0.32          |
| (1,659)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HA    | 4        | 0.32          |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 9        | 0.32          |
| (1,484)  | 1:59:A:THR:HG23  | 1:62:A:GLN:HG2   | 2        | 0.32          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 9        | 0.32          |
| (1,304)  | 1:72:A:THR:HG23  | 1:73:A:THR:H     | 2        | 0.32          |
| (1,298)  | 1:101:A:VAL:HG11 | 1:110:A:ASP:HB2  | 6        | 0.32          |
| (1,258)  | 1:76:A:GLU:HB2   | 1:72:A:THR:HA    | 7        | 0.32          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 1        | 0.32          |
| (1,207)  | 1:122:A:THR:HB   | 1:123:A:ASP:HB3  | 9        | 0.32          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 2        | 0.32          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 6        | 0.32          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 7        | 0.32          |
| (1,199)  | 1:111:A:VAL:HG11 | 1:112:A:PHE:H    | 3        | 0.32          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 4        | 0.32          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 9        | 0.32          |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD12  | 8        | 0.32          |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG22  | 7        | 0.32          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD13  | 7        | 0.32          |
| (1,1577) | 1:85:A:TYR:H     | 1:68:A:VAL:H     | 3        | 0.31          |
| (1,1479) | 1:52:A:LEU:HG    | 1:49:A:MET:HA    | 5        | 0.31          |
| (1,1470) | 1:86:A:ILE:HG21  | 1:85:A:TYR:H     | 2        | 0.31          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 8        | 0.31          |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG2   | 9        | 0.31          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 6        | 0.31          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 8        | 0.31          |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 10       | 0.31          |
| (1,1245) | 1:40:A:ILE:HD11  | 1:37:A:ILE:H     | 9        | 0.31          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 2        | 0.31          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 5        | 0.31          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB2   | 9        | 0.31          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 7        | 0.31          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 10       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1091) | 1:32:A:ASP:H     | 1:28:A:LYS:HG3   | 10       | 0.31          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 7        | 0.31          |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 2        | 0.31          |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 4        | 0.31          |
| (1,1062) | 1:100:A:LEU:HD21 | 1:64:A:LEU:H     | 2        | 0.31          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG23 | 8        | 0.31          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 2        | 0.31          |
| (1,904)  | 1:106:A:HIS:HB3  | 1:107:A:GLY:H    | 2        | 0.31          |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 7        | 0.31          |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 9        | 0.31          |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 10       | 0.31          |
| (1,810)  | 1:36:A:ALA:HA    | 1:113:A:SER:HB2  | 7        | 0.31          |
| (1,772)  | 1:105:A:ARG:HG2  | 1:106:A:HIS:HD2  | 6        | 0.31          |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD2  | 2        | 0.31          |
| (1,766)  | 1:131:A:VAL:HG22 | 1:128:A:ASN:HB3  | 1        | 0.31          |
| (1,764)  | 1:44:A:GLU:HG2   | 1:128:A:ASN:HD21 | 5        | 0.31          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 2        | 0.31          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 10       | 0.31          |
| (1,676)  | 1:109:A:VAL:HG22 | 1:100:A:LEU:HA   | 10       | 0.31          |
| (1,659)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HA    | 10       | 0.31          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 3        | 0.31          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 4        | 0.31          |
| (1,616)  | 1:100:A:LEU:HD23 | 1:58:A:PRO:HG2   | 6        | 0.31          |
| (1,616)  | 1:100:A:LEU:HD22 | 1:58:A:PRO:HG2   | 9        | 0.31          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG21  | 8        | 0.31          |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG23  | 2        | 0.31          |
| (1,421)  | 1:129:A:TRP:HB2  | 1:106:A:HIS:HB2  | 5        | 0.31          |
| (1,359)  | 1:64:A:LEU:HD11  | 1:67:A:LEU:H     | 9        | 0.31          |
| (1,336)  | 1:52:A:LEU:HD13  | 1:48:A:ASP:HB3   | 10       | 0.31          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 3        | 0.31          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 9        | 0.31          |
| (1,201)  | 1:111:A:VAL:HG11 | 1:128:A:ASN:HD21 | 1        | 0.31          |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 6        | 0.31          |
| (1,182)  | 1:32:A:ASP:HB3   | 1:93:A:PRO:HB2   | 4        | 0.31          |
| (1,134)  | 1:122:A:THR:HG22 | 1:123:A:ASP:H    | 5        | 0.31          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 10       | 0.31          |
| (1,95)   | 1:37:A:ILE:HG22  | 1:41:A:VAL:H     | 10       | 0.31          |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD11  | 4        | 0.31          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD11  | 4        | 0.31          |
| (1,1590) | 1:55:A:SER:H     | 1:51:A:LYS:HB2   | 10       | 0.3           |
| (1,1580) | 1:48:A:ASP:H     | 1:52:A:LEU:HD22  | 9        | 0.3           |
| (1,1569) | 1:92:A:ASP:H     | 1:95:A:GLY:H     | 4        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1504) | 1:96:A:ALA:HB3   | 1:95:A:GLY:H     | 2        | 0.3           |
| (1,1504) | 1:96:A:ALA:HB2   | 1:95:A:GLY:H     | 9        | 0.3           |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 3        | 0.3           |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 3        | 0.3           |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2   | 7        | 0.3           |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 2        | 0.3           |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 2        | 0.3           |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 6        | 0.3           |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 3        | 0.3           |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 7        | 0.3           |
| (1,1247) | 1:57:A:TYR:H     | 1:109:A:VAL:HG11 | 5        | 0.3           |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB1   | 9        | 0.3           |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2   | 4        | 0.3           |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 9        | 0.3           |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 3        | 0.3           |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 5        | 0.3           |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 6        | 0.3           |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 7        | 0.3           |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 8        | 0.3           |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 9        | 0.3           |
| (1,1079) | 1:62:A:GLN:HE21  | 1:62:A:GLN:HG2   | 10       | 0.3           |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG13 | 6        | 0.3           |
| (1,1041) | 1:100:A:LEU:HB2  | 1:100:A:LEU:H    | 6        | 0.3           |
| (1,1028) | 1:86:A:ILE:H     | 1:46:A:ALA:HB3   | 8        | 0.3           |
| (1,1007) | 1:109:A:VAL:H    | 1:108:A:LYS:HD2  | 3        | 0.3           |
| (1,978)  | 1:98:A:TYR:HB3   | 1:98:A:TYR:H     | 8        | 0.3           |
| (1,978)  | 1:98:A:TYR:HB3   | 1:98:A:TYR:H     | 10       | 0.3           |
| (1,904)  | 1:106:A:HIS:HB3  | 1:107:A:GLY:H    | 10       | 0.3           |
| (1,810)  | 1:36:A:ALA:HA    | 1:113:A:SER:HB2  | 3        | 0.3           |
| (1,772)  | 1:105:A:ARG:HG2  | 1:106:A:HIS:HD2  | 8        | 0.3           |
| (1,767)  | 1:122:A:THR:HG22 | 1:121:A:ASP:H    | 7        | 0.3           |
| (1,767)  | 1:122:A:THR:HG22 | 1:121:A:ASP:H    | 9        | 0.3           |
| (1,763)  | 1:44:A:GLU:HG2   | 1:45:A:SER:H     | 2        | 0.3           |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 6        | 0.3           |
| (1,738)  | 1:78:A:ARG:HD2   | 1:54:A:ASN:H     | 5        | 0.3           |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 7        | 0.3           |
| (1,676)  | 1:109:A:VAL:HG21 | 1:100:A:LEU:HA   | 9        | 0.3           |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG22 | 5        | 0.3           |
| (1,659)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HA    | 7        | 0.3           |
| (1,657)  | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD11  | 1        | 0.3           |
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB1   | 4        | 0.3           |
| (1,618)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:H    | 4        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG22  | 1        | 0.3           |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG23  | 6        | 0.3           |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG21  | 10       | 0.3           |
| (1,484)  | 1:59:A:THR:HG22  | 1:62:A:GLN:HG2   | 8        | 0.3           |
| (1,300)  | 1:73:A:THR:HG22  | 1:71:A:PRO:HB3   | 3        | 0.3           |
| (1,298)  | 1:101:A:VAL:HG12 | 1:110:A:ASP:HB2  | 1        | 0.3           |
| (1,253)  | 1:92:A:ASP:HB2   | 1:113:A:SER:HB3  | 7        | 0.3           |
| (1,241)  | 1:105:A:ARG:HA   | 1:104:A:GLY:HA2  | 9        | 0.3           |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 2        | 0.3           |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 8        | 0.3           |
| (1,228)  | 1:63:A:GLY:HA2   | 1:100:A:LEU:HB2  | 3        | 0.3           |
| (1,222)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HB2   | 10       | 0.3           |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 9        | 0.3           |
| (1,165)  | 1:30:A:LYS:HA    | 1:30:A:LYS:HB2   | 3        | 0.3           |
| (1,154)  | 1:80:A:TYR:HB2   | 1:77:A:PRO:HB2   | 4        | 0.3           |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 7        | 0.3           |
| (1,95)   | 1:37:A:ILE:HG22  | 1:41:A:VAL:H     | 9        | 0.3           |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD13  | 3        | 0.3           |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG21  | 5        | 0.3           |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB3   | 6        | 0.3           |
| (1,12)   | 1:105:A:ARG:HD2  | 1:105:A:ARG:HA   | 10       | 0.3           |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB2   | 1        | 0.29          |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG21  | 10       | 0.29          |
| (1,1523) | 1:140:A:SER:HB3  | 1:139:A:GLY:H    | 7        | 0.29          |
| (1,1504) | 1:96:A:ALA:HB1   | 1:95:A:GLY:H     | 6        | 0.29          |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 6        | 0.29          |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 7        | 0.29          |
| (1,1479) | 1:52:A:LEU:HG    | 1:49:A:MET:HA    | 10       | 0.29          |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE1   | 1        | 0.29          |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE2   | 7        | 0.29          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 6        | 0.29          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 9        | 0.29          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 2        | 0.29          |
| (1,1269) | 1:55:A:SER:H     | 1:51:A:LYS:HD3   | 8        | 0.29          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 6        | 0.29          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 8        | 0.29          |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB2   | 1        | 0.29          |
| (1,1154) | 1:92:A:ASP:H     | 1:96:A:ALA:HB1   | 5        | 0.29          |
| (1,1146) | 1:105:A:ARG:HB3  | 1:105:A:ARG:H    | 2        | 0.29          |
| (1,1099) | 1:99:A:GLN:H     | 1:111:A:VAL:HG13 | 9        | 0.29          |
| (1,1041) | 1:100:A:LEU:HB2  | 1:100:A:LEU:H    | 7        | 0.29          |
| (1,998)  | 1:43:A:LEU:HD12  | 1:43:A:LEU:H     | 3        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,998)  | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 4        | 0.29          |
| (1,998)  | 1:43:A:LEU:HD12  | 1:43:A:LEU:H     | 8        | 0.29          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 8        | 0.29          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 3        | 0.29          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 6        | 0.29          |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 3        | 0.29          |
| (1,767)  | 1:122:A:THR:HG22 | 1:121:A:ASP:H    | 4        | 0.29          |
| (1,744)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB3   | 6        | 0.29          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 3        | 0.29          |
| (1,676)  | 1:109:A:VAL:HG22 | 1:100:A:LEU:HA   | 3        | 0.29          |
| (1,659)  | 1:111:A:VAL:HG22 | 1:40:A:ILE:HA    | 2        | 0.29          |
| (1,659)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HA    | 5        | 0.29          |
| (1,659)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HA    | 9        | 0.29          |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD21 | 4        | 0.29          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG22  | 7        | 0.29          |
| (1,561)  | 1:135:A:ALA:HB3  | 1:138:A:ASN:HA   | 2        | 0.29          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 5        | 0.29          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 6        | 0.29          |
| (1,484)  | 1:59:A:THR:HG22  | 1:62:A:GLN:HG2   | 6        | 0.29          |
| (1,360)  | 1:64:A:LEU:HD11  | 1:68:A:VAL:H     | 9        | 0.29          |
| (1,298)  | 1:101:A:VAL:HG13 | 1:110:A:ASP:HB2  | 8        | 0.29          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 4        | 0.29          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 5        | 0.29          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 6        | 0.29          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 10       | 0.29          |
| (1,199)  | 1:111:A:VAL:HG13 | 1:112:A:PHE:H    | 8        | 0.29          |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 3        | 0.29          |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB3   | 4        | 0.29          |
| (1,136)  | 1:50:A:TYR:HA    | 1:54:A:ASN:HB2   | 7        | 0.29          |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD13  | 7        | 0.29          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 1        | 0.29          |
| (1,1504) | 1:96:A:ALA:HB2   | 1:95:A:GLY:H     | 3        | 0.28          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 4        | 0.28          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 6        | 0.28          |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 1        | 0.28          |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 4        | 0.28          |
| (1,1479) | 1:52:A:LEU:HG    | 1:49:A:MET:HA    | 9        | 0.28          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD1   | 5        | 0.28          |
| (1,1399) | 1:51:A:LYS:H     | 1:57:A:TYR:HE2   | 6        | 0.28          |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG2   | 4        | 0.28          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 9        | 0.28          |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 2        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD3   | 7        | 0.28          |
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 6        | 0.28          |
| (1,998)  | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 5        | 0.28          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 9        | 0.28          |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 2        | 0.28          |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 7        | 0.28          |
| (1,810)  | 1:36:A:ALA:HA    | 1:113:A:SER:HB2  | 8        | 0.28          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 1        | 0.28          |
| (1,801)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HB2   | 9        | 0.28          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 9        | 0.28          |
| (1,699)  | 1:101:A:VAL:HG22 | 1:105:A:ARG:HD2  | 10       | 0.28          |
| (1,664)  | 1:109:A:VAL:HG22 | 1:109:A:VAL:HA   | 3        | 0.28          |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2   | 2        | 0.28          |
| (1,659)  | 1:111:A:VAL:HG23 | 1:40:A:ILE:HA    | 1        | 0.28          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 8        | 0.28          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 9        | 0.28          |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD23 | 5        | 0.28          |
| (1,579)  | 1:93:A:PRO:HG2   | 1:94:A:TRP:H     | 7        | 0.28          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG22  | 4        | 0.28          |
| (1,553)  | 1:85:A:TYR:HB3   | 1:85:A:TYR:H     | 9        | 0.28          |
| (1,544)  | 1:57:A:TYR:HA    | 1:57:A:TYR:HD2   | 10       | 0.28          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 5        | 0.28          |
| (1,387)  | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 5        | 0.28          |
| (1,387)  | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 7        | 0.28          |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD21  | 1        | 0.28          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG21  | 1        | 0.28          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG23  | 5        | 0.28          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG23  | 7        | 0.28          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG22  | 9        | 0.28          |
| (1,253)  | 1:92:A:ASP:HB2   | 1:113:A:SER:HB3  | 3        | 0.28          |
| (1,231)  | 1:63:A:GLY:HA2   | 1:64:A:LEU:H     | 7        | 0.28          |
| (1,220)  | 1:107:A:GLY:HA3  | 1:108:A:LYS:HD2  | 5        | 0.28          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 8        | 0.28          |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 10       | 0.28          |
| (1,95)   | 1:37:A:ILE:HG22  | 1:41:A:VAL:H     | 8        | 0.28          |
| (1,83)   | 1:36:A:ALA:HB1   | 1:94:A:TRP:HH2   | 4        | 0.28          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 3        | 0.28          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB1   | 4        | 0.28          |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG12 | 7        | 0.28          |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG11 | 10       | 0.28          |
| (1,1590) | 1:55:A:SER:H     | 1:51:A:LYS:HB2   | 1        | 0.27          |
| (1,1569) | 1:92:A:ASP:H     | 1:95:A:GLY:H     | 7        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1506) | 1:66:A:ALA:HB3   | 1:71:A:PRO:HB2   | 7        | 0.27          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 1        | 0.27          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 5        | 0.27          |
| (1,1462) | 1:45:A:SER:HB2   | 1:44:A:GLU:HB3   | 1        | 0.27          |
| (1,1457) | 1:41:A:VAL:HB    | 1:133:A:THR:H    | 4        | 0.27          |
| (1,1439) | 1:79:A:SER:H     | 1:78:A:ARG:HD3   | 9        | 0.27          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD1   | 1        | 0.27          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD2   | 7        | 0.27          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD1   | 9        | 0.27          |
| (1,1415) | 1:33:A:ARG:H     | 1:30:A:LYS:HB3   | 3        | 0.27          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 7        | 0.27          |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG3   | 5        | 0.27          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 3        | 0.27          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 1        | 0.27          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 3        | 0.27          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 4        | 0.27          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 5        | 0.27          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 7        | 0.27          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 10       | 0.27          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD13  | 1        | 0.27          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD11  | 4        | 0.27          |
| (1,1236) | 1:34:A:GLN:H     | 1:30:A:LYS:HB3   | 8        | 0.27          |
| (1,1143) | 1:106:A:HIS:H    | 1:105:A:ARG:HB3  | 4        | 0.27          |
| (1,1126) | 1:51:A:LYS:H     | 1:51:A:LYS:HD2   | 4        | 0.27          |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG13 | 7        | 0.27          |
| (1,998)  | 1:43:A:LEU:HD11  | 1:43:A:LEU:H     | 1        | 0.27          |
| (1,998)  | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 2        | 0.27          |
| (1,998)  | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 6        | 0.27          |
| (1,998)  | 1:43:A:LEU:HD12  | 1:43:A:LEU:H     | 9        | 0.27          |
| (1,998)  | 1:43:A:LEU:HD11  | 1:43:A:LEU:H     | 10       | 0.27          |
| (1,987)  | 1:117:A:ASP:H    | 1:119:A:MET:H    | 8        | 0.27          |
| (1,888)  | 1:108:A:LYS:HB3  | 1:108:A:LYS:H    | 5        | 0.27          |
| (1,848)  | 1:70:A:LYS:H     | 1:70:A:LYS:HG3   | 1        | 0.27          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 2        | 0.27          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 4        | 0.27          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 6        | 0.27          |
| (1,766)  | 1:131:A:VAL:HG22 | 1:128:A:ASN:HB3  | 2        | 0.27          |
| (1,764)  | 1:44:A:GLU:HG2   | 1:128:A:ASN:HD21 | 4        | 0.27          |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 7        | 0.27          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 8        | 0.27          |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 4        | 0.27          |
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB1   | 1        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB2   | 8        | 0.27          |
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB3   | 9        | 0.27          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 1        | 0.27          |
| (1,592)  | 1:88:A:ARG:HD2   | 1:88:A:ARG:HA    | 6        | 0.27          |
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 1        | 0.27          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG22  | 5        | 0.27          |
| (1,484)  | 1:59:A:THR:HG21  | 1:62:A:GLN:HG2   | 10       | 0.27          |
| (1,469)  | 1:44:A:GLU:HG3   | 1:44:A:GLU:HA    | 4        | 0.27          |
| (1,391)  | 1:133:A:THR:HA   | 1:134:A:SER:H    | 9        | 0.27          |
| (1,387)  | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 10       | 0.27          |
| (1,336)  | 1:52:A:LEU:HD21  | 1:48:A:ASP:HB3   | 2        | 0.27          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 4        | 0.27          |
| (1,300)  | 1:73:A:THR:HG22  | 1:71:A:PRO:HB3   | 9        | 0.27          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG23  | 3        | 0.27          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 4        | 0.27          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 5        | 0.27          |
| (1,95)   | 1:37:A:ILE:HG23  | 1:41:A:VAL:H     | 4        | 0.27          |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD12  | 9        | 0.27          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 10       | 0.27          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB3   | 1        | 0.27          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB3   | 10       | 0.27          |
| (1,38)   | 1:33:A:ARG:HA    | 1:37:A:ILE:HD12  | 8        | 0.27          |
| (1,4)    | 1:126:A:ILE:HG22 | 1:126:A:ILE:H    | 9        | 0.27          |
| (1,1587) | 1:127:A:GLY:H    | 1:40:A:ILE:HG22  | 7        | 0.26          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD11  | 3        | 0.26          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 3        | 0.26          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 7        | 0.26          |
| (1,1472) | 1:78:A:ARG:HD3   | 1:78:A:ARG:HB2   | 7        | 0.26          |
| (1,1470) | 1:86:A:ILE:HG23  | 1:85:A:TYR:H     | 4        | 0.26          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD2   | 3        | 0.26          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 4        | 0.26          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 9        | 0.26          |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2   | 2        | 0.26          |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2   | 5        | 0.26          |
| (1,1380) | 1:132:A:GLY:HA3  | 1:40:A:ILE:H     | 10       | 0.26          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 4        | 0.26          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD12  | 5        | 0.26          |
| (1,1123) | 1:30:A:LYS:H     | 1:30:A:LYS:HG3   | 2        | 0.26          |
| (1,1028) | 1:86:A:ILE:H     | 1:46:A:ALA:HB2   | 2        | 0.26          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 7        | 0.26          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 8        | 0.26          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 4        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 7        | 0.26          |
| (1,764)  | 1:44:A:GLU:HG2   | 1:128:A:ASN:HD21 | 10       | 0.26          |
| (1,763)  | 1:44:A:GLU:HG2   | 1:45:A:SER:H     | 1        | 0.26          |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 5        | 0.26          |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 10       | 0.26          |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 6        | 0.26          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 6        | 0.26          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 3        | 0.26          |
| (1,676)  | 1:109:A:VAL:HG23 | 1:100:A:LEU:HA   | 8        | 0.26          |
| (1,657)  | 1:111:A:VAL:HG23 | 1:43:A:LEU:HD13  | 6        | 0.26          |
| (1,634)  | 1:79:A:SER:HB3   | 1:54:A:ASN:HA    | 10       | 0.26          |
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB3   | 5        | 0.26          |
| (1,630)  | 1:32:A:ASP:HB3   | 1:31:A:ALA:HB2   | 6        | 0.26          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 2        | 0.26          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 5        | 0.26          |
| (1,618)  | 1:100:A:LEU:HD21 | 1:100:A:LEU:H    | 3        | 0.26          |
| (1,610)  | 1:66:A:ALA:HB3   | 1:62:A:GLN:HE21  | 4        | 0.26          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG21  | 9        | 0.26          |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG22  | 6        | 0.26          |
| (1,407)  | 1:61:A:GLU:HA    | 1:61:A:GLU:HG3   | 9        | 0.26          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG22 | 5        | 0.26          |
| (1,336)  | 1:52:A:LEU:HD21  | 1:48:A:ASP:HB3   | 3        | 0.26          |
| (1,300)  | 1:73:A:THR:HG21  | 1:71:A:PRO:HB3   | 10       | 0.26          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG21  | 2        | 0.26          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG23  | 6        | 0.26          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG21  | 8        | 0.26          |
| (1,253)  | 1:92:A:ASP:HB2   | 1:113:A:SER:HB3  | 8        | 0.26          |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 7        | 0.26          |
| (1,95)   | 1:37:A:ILE:HG23  | 1:41:A:VAL:H     | 7        | 0.26          |
| (1,90)   | 1:34:A:GLN:HG2   | 1:37:A:ILE:HD12  | 5        | 0.26          |
| (1,83)   | 1:36:A:ALA:HB3   | 1:94:A:TRP:HH2   | 10       | 0.26          |
| (1,57)   | 1:34:A:GLN:HA    | 1:37:A:ILE:H     | 3        | 0.26          |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG22  | 10       | 0.26          |
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H     | 8        | 0.26          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB2   | 2        | 0.26          |
| (1,1582) | 1:115:A:GLY:H    | 1:114:A:TYR:HD2  | 10       | 0.25          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD13  | 1        | 0.25          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD12  | 4        | 0.25          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD13  | 10       | 0.25          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 4        | 0.25          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 4        | 0.25          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 9        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 10       | 0.25          |
| (1,1479) | 1:52:A:LEU:HG    | 1:49:A:MET:HA    | 6        | 0.25          |
| (1,1462) | 1:45:A:SER:HB2   | 1:44:A:GLU:HB3   | 10       | 0.25          |
| (1,1457) | 1:41:A:VAL:HB    | 1:133:A:THR:H    | 10       | 0.25          |
| (1,1452) | 1:37:A:ILE:HA    | 1:37:A:ILE:HD13  | 9        | 0.25          |
| (1,1411) | 1:66:A:ALA:HB1   | 1:68:A:VAL:H     | 3        | 0.25          |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 2        | 0.25          |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 5        | 0.25          |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 7        | 0.25          |
| (1,1318) | 1:42:A:ALA:H     | 1:88:A:ARG:HD3   | 5        | 0.25          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 6        | 0.25          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 8        | 0.25          |
| (1,1289) | 1:45:A:SER:H     | 1:43:A:LEU:HG    | 9        | 0.25          |
| (1,1261) | 1:109:A:VAL:HG11 | 1:128:A:ASN:HD21 | 2        | 0.25          |
| (1,1261) | 1:109:A:VAL:HG13 | 1:128:A:ASN:HD21 | 9        | 0.25          |
| (1,1257) | 1:127:A:GLY:H    | 1:40:A:ILE:HD13  | 10       | 0.25          |
| (1,1204) | 1:48:A:ASP:H     | 1:46:A:ALA:HB2   | 6        | 0.25          |
| (1,998)  | 1:43:A:LEU:HD13  | 1:43:A:LEU:H     | 7        | 0.25          |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG22 | 7        | 0.25          |
| (1,880)  | 1:29:A:GLU:H     | 1:29:A:GLU:HG3   | 6        | 0.25          |
| (1,779)  | 1:40:A:ILE:HG21  | 1:112:A:PHE:HA   | 8        | 0.25          |
| (1,779)  | 1:40:A:ILE:HG23  | 1:112:A:PHE:HA   | 10       | 0.25          |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD2  | 9        | 0.25          |
| (1,767)  | 1:122:A:THR:HG23 | 1:121:A:ASP:H    | 10       | 0.25          |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 2        | 0.25          |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 3        | 0.25          |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 7        | 0.25          |
| (1,738)  | 1:78:A:ARG:HD3   | 1:54:A:ASN:H     | 10       | 0.25          |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 1        | 0.25          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 1        | 0.25          |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG21 | 4        | 0.25          |
| (1,659)  | 1:111:A:VAL:HG21 | 1:40:A:ILE:HA    | 8        | 0.25          |
| (1,658)  | 1:111:A:VAL:HG22 | 1:44:A:GLU:HA    | 1        | 0.25          |
| (1,658)  | 1:111:A:VAL:HG21 | 1:44:A:GLU:HA    | 4        | 0.25          |
| (1,658)  | 1:111:A:VAL:HG23 | 1:44:A:GLU:HA    | 8        | 0.25          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB2   | 3        | 0.25          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB2   | 5        | 0.25          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB2   | 9        | 0.25          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB2   | 10       | 0.25          |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD22 | 1        | 0.25          |
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 5        | 0.25          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG21  | 2        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 10       | 0.25          |
| (1,512)  | 1:91:A:GLN:HB3   | 1:92:A:ASP:H     | 7        | 0.25          |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG22  | 4        | 0.25          |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG22  | 7        | 0.25          |
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG23  | 2        | 0.25          |
| (1,449)  | 1:109:A:VAL:HG13 | 1:108:A:LYS:HD3  | 10       | 0.25          |
| (1,387)  | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 1        | 0.25          |
| (1,387)  | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 9        | 0.25          |
| (1,336)  | 1:52:A:LEU:HD22  | 1:48:A:ASP:HB3   | 1        | 0.25          |
| (1,336)  | 1:52:A:LEU:HD23  | 1:48:A:ASP:HB3   | 8        | 0.25          |
| (1,300)  | 1:73:A:THR:HG21  | 1:71:A:PRO:HB3   | 7        | 0.25          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG23  | 4        | 0.25          |
| (1,296)  | 1:72:A:THR:HB    | 1:72:A:THR:HG22  | 10       | 0.25          |
| (1,258)  | 1:76:A:GLU:HB2   | 1:72:A:THR:HA    | 9        | 0.25          |
| (1,255)  | 1:43:A:LEU:HB3   | 1:40:A:ILE:HA    | 1        | 0.25          |
| (1,201)  | 1:111:A:VAL:HG12 | 1:128:A:ASN:HD21 | 9        | 0.25          |
| (1,143)  | 1:133:A:THR:HB   | 1:134:A:SER:H    | 8        | 0.25          |
| (1,136)  | 1:50:A:TYR:HA    | 1:54:A:ASN:HB2   | 2        | 0.25          |
| (1,136)  | 1:50:A:TYR:HA    | 1:54:A:ASN:HB3   | 3        | 0.25          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 2        | 0.25          |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG21  | 8        | 0.25          |
| (1,21)   | 1:31:A:ALA:HA    | 1:30:A:LYS:HB3   | 2        | 0.25          |
| (1,14)   | 1:28:A:LYS:HG3   | 1:28:A:LYS:HE2   | 7        | 0.25          |
| (1,12)   | 1:105:A:ARG:HD2  | 1:105:A:ARG:HA   | 2        | 0.25          |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG12 | 5        | 0.25          |
| (1,4)    | 1:126:A:ILE:HG22 | 1:126:A:ILE:H    | 2        | 0.25          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 4        | 0.24          |
| (1,1567) | 1:68:A:VAL:H     | 1:86:A:ILE:HD11  | 6        | 0.24          |
| (1,1537) | 1:49:A:MET:H     | 1:136:A:HIS:HD2  | 4        | 0.24          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 2        | 0.24          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 8        | 0.24          |
| (1,1501) | 1:109:A:VAL:HB   | 1:109:A:VAL:H    | 10       | 0.24          |
| (1,1484) | 1:64:A:LEU:HD22  | 1:63:A:GLY:HA2   | 5        | 0.24          |
| (1,1444) | 1:27:A:ASN:HB2   | 1:30:A:LYS:HB3   | 9        | 0.24          |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG3   | 3        | 0.24          |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG2   | 10       | 0.24          |
| (1,1353) | 1:138:A:ASN:HD21 | 1:138:A:ASN:HA   | 1        | 0.24          |
| (1,1345) | 1:126:A:ILE:H    | 1:113:A:SER:HB2  | 6        | 0.24          |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 6        | 0.24          |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 9        | 0.24          |
| (1,1180) | 1:118:A:GLY:H    | 1:119:A:MET:HB3  | 9        | 0.24          |
| (1,1091) | 1:32:A:ASP:H     | 1:28:A:LYS:HG2   | 7        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 4        | 0.24          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 6        | 0.24          |
| (1,920)  | 1:87:A:ARG:HB3   | 1:88:A:ARG:H     | 7        | 0.24          |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG22 | 4        | 0.24          |
| (1,915)  | 1:122:A:THR:H    | 1:121:A:ASP:HB3  | 3        | 0.24          |
| (1,880)  | 1:29:A:GLU:H     | 1:29:A:GLU:HG3   | 9        | 0.24          |
| (1,848)  | 1:70:A:LYS:H     | 1:70:A:LYS:HG2   | 8        | 0.24          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 10       | 0.24          |
| (1,784)  | 1:114:A:TYR:HA   | 1:126:A:ILE:HB   | 8        | 0.24          |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD2  | 3        | 0.24          |
| (1,745)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HD22 | 2        | 0.24          |
| (1,744)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB3   | 2        | 0.24          |
| (1,744)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB3   | 8        | 0.24          |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 1        | 0.24          |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 8        | 0.24          |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE1  | 7        | 0.24          |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 5        | 0.24          |
| (1,720)  | 1:108:A:LYS:HA   | 1:103:A:PRO:HB3  | 7        | 0.24          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 4        | 0.24          |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG22 | 10       | 0.24          |
| (1,658)  | 1:111:A:VAL:HG22 | 1:44:A:GLU:HA    | 3        | 0.24          |
| (1,650)  | 1:32:A:ASP:HB2   | 1:93:A:PRO:HB2   | 3        | 0.24          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB3   | 1        | 0.24          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB1   | 2        | 0.24          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB2   | 4        | 0.24          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB1   | 6        | 0.24          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB1   | 7        | 0.24          |
| (1,632)  | 1:79:A:SER:HB3   | 1:78:A:ARG:HG3   | 4        | 0.24          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 7        | 0.24          |
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 4        | 0.24          |
| (1,567)  | 1:131:A:VAL:HA   | 1:37:A:ILE:HG23  | 3        | 0.24          |
| (1,525)  | 1:61:A:GLU:HG2   | 1:73:A:THR:HG23  | 1        | 0.24          |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG22  | 3        | 0.24          |
| (1,474)  | 1:69:A:LYS:HB2   | 1:68:A:VAL:HB    | 5        | 0.24          |
| (1,474)  | 1:69:A:LYS:HB2   | 1:68:A:VAL:HB    | 10       | 0.24          |
| (1,469)  | 1:44:A:GLU:HG3   | 1:44:A:GLU:HA    | 8        | 0.24          |
| (1,434)  | 1:41:A:VAL:HG11  | 1:38:A:SER:H     | 6        | 0.24          |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD21  | 9        | 0.24          |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD22  | 10       | 0.24          |
| (1,337)  | 1:52:A:LEU:HD12  | 1:52:A:LEU:HB3   | 6        | 0.24          |
| (1,336)  | 1:52:A:LEU:HD21  | 1:48:A:ASP:HB3   | 4        | 0.24          |
| (1,300)  | 1:73:A:THR:HG23  | 1:71:A:PRO:HB3   | 2        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,300)  | 1:73:A:THR:HG23  | 1:71:A:PRO:HB3   | 4        | 0.24          |
| (1,275)  | 1:119:A:MET:HB3  | 1:122:A:THR:HG22 | 7        | 0.24          |
| (1,253)  | 1:92:A:ASP:HB3   | 1:113:A:SER:HB3  | 5        | 0.24          |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 5        | 0.24          |
| (1,143)  | 1:133:A:THR:HB   | 1:134:A:SER:H    | 4        | 0.24          |
| (1,131)  | 1:41:A:VAL:HB    | 1:45:A:SER:HB2   | 5        | 0.24          |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG23  | 9        | 0.24          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB3   | 5        | 0.24          |
| (1,29)   | 1:105:A:ARG:HA   | 1:105:A:ARG:HB3  | 6        | 0.24          |
| (1,4)    | 1:126:A:ILE:HG22 | 1:126:A:ILE:H    | 3        | 0.24          |
| (1,2)    | 1:80:A:TYR:HB3   | 1:85:A:TYR:HD2   | 8        | 0.24          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 3        | 0.23          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 6        | 0.23          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 10       | 0.23          |
| (1,1569) | 1:92:A:ASP:H     | 1:95:A:GLY:H     | 5        | 0.23          |
| (1,1481) | 1:131:A:VAL:HB   | 1:37:A:ILE:HD13  | 1        | 0.23          |
| (1,1481) | 1:37:A:ILE:HG22  | 1:131:A:VAL:HB   | 4        | 0.23          |
| (1,1457) | 1:41:A:VAL:HB    | 1:133:A:THR:H    | 6        | 0.23          |
| (1,1452) | 1:37:A:ILE:HA    | 1:37:A:ILE:HD12  | 2        | 0.23          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD2   | 6        | 0.23          |
| (1,1411) | 1:66:A:ALA:HB2   | 1:68:A:VAL:H     | 10       | 0.23          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 5        | 0.23          |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG3   | 6        | 0.23          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 5        | 0.23          |
| (1,1345) | 1:126:A:ILE:H    | 1:113:A:SER:HB2  | 4        | 0.23          |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 3        | 0.23          |
| (1,1254) | 1:124:A:ASP:H    | 1:122:A:THR:HG22 | 3        | 0.23          |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 1        | 0.23          |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 3        | 0.23          |
| (1,1160) | 1:96:A:ALA:HB3   | 1:95:A:GLY:H     | 8        | 0.23          |
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 7        | 0.23          |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG13 | 8        | 0.23          |
| (1,1006) | 1:108:A:LYS:HB2  | 1:109:A:VAL:H    | 6        | 0.23          |
| (1,993)  | 1:34:A:GLN:HE22  | 1:37:A:ILE:HD11  | 10       | 0.23          |
| (1,987)  | 1:117:A:ASP:H    | 1:119:A:MET:H    | 2        | 0.23          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 3        | 0.23          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 4        | 0.23          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 9        | 0.23          |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG21 | 8        | 0.23          |
| (1,880)  | 1:29:A:GLU:H     | 1:29:A:GLU:HG3   | 8        | 0.23          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 3        | 0.23          |
| (1,806)  | 1:37:A:ILE:HG21  | 1:34:A:GLN:HE22  | 4        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,803)  | 1:46:A:ALA:HB3   | 1:67:A:LEU:HA    | 5        | 0.23          |
| (1,763)  | 1:44:A:GLU:HG2   | 1:45:A:SER:H     | 7        | 0.23          |
| (1,742)  | 1:31:A:ALA:HA    | 1:33:A:ARG:HG2   | 9        | 0.23          |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 4        | 0.23          |
| (1,722)  | 1:51:A:LYS:HA    | 1:54:A:ASN:HA    | 4        | 0.23          |
| (1,720)  | 1:108:A:LYS:HA   | 1:103:A:PRO:HB3  | 1        | 0.23          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 2        | 0.23          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 9        | 0.23          |
| (1,670)  | 1:111:A:VAL:HG11 | 1:109:A:VAL:HG23 | 1        | 0.23          |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG23 | 8        | 0.23          |
| (1,658)  | 1:111:A:VAL:HG22 | 1:44:A:GLU:HA    | 9        | 0.23          |
| (1,621)  | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 10       | 0.23          |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD21 | 3        | 0.23          |
| (1,610)  | 1:66:A:ALA:HB1   | 1:62:A:GLN:HE21  | 5        | 0.23          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 3        | 0.23          |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG23  | 8        | 0.23          |
| (1,484)  | 1:59:A:THR:HG21  | 1:62:A:GLN:HG2   | 7        | 0.23          |
| (1,466)  | 1:82:A:GLN:HG2   | 1:83:A:ASP:H     | 8        | 0.23          |
| (1,435)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:H     | 1        | 0.23          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 8        | 0.23          |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG22  | 8        | 0.23          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG22 | 3        | 0.23          |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD21  | 4        | 0.23          |
| (1,351)  | 1:140:A:SER:HB3  | 1:138:A:ASN:HB3  | 4        | 0.23          |
| (1,339)  | 1:52:A:LEU:HD13  | 1:136:A:HIS:HD2  | 1        | 0.23          |
| (1,337)  | 1:52:A:LEU:HD13  | 1:52:A:LEU:HB3   | 9        | 0.23          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 9        | 0.23          |
| (1,300)  | 1:73:A:THR:HG22  | 1:71:A:PRO:HB3   | 1        | 0.23          |
| (1,298)  | 1:101:A:VAL:HG12 | 1:110:A:ASP:HB2  | 2        | 0.23          |
| (1,282)  | 1:78:A:ARG:HD2   | 1:78:A:ARG:HG3   | 1        | 0.23          |
| (1,282)  | 1:78:A:ARG:HD3   | 1:78:A:ARG:HG2   | 10       | 0.23          |
| (1,253)  | 1:92:A:ASP:HB2   | 1:113:A:SER:HB3  | 2        | 0.23          |
| (1,222)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HB2   | 4        | 0.23          |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 1        | 0.23          |
| (1,39)   | 1:33:A:ARG:HA    | 1:36:A:ALA:HB1   | 9        | 0.23          |
| (1,21)   | 1:31:A:ALA:HA    | 1:30:A:LYS:HB3   | 10       | 0.23          |
| (1,12)   | 1:105:A:ARG:HD3  | 1:105:A:ARG:HA   | 3        | 0.23          |
| (1,5)    | 1:126:A:ILE:HG23 | 1:37:A:ILE:HA    | 6        | 0.23          |
| (1,1595) | 1:32:A:ASP:H     | 1:30:A:LYS:HB3   | 5        | 0.22          |
| (1,1587) | 1:127:A:GLY:H    | 1:40:A:ILE:HD12  | 6        | 0.22          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 1        | 0.22          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 5        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 7        | 0.22          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 8        | 0.22          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 9        | 0.22          |
| (1,1577) | 1:85:A:TYR:H     | 1:68:A:VAL:H     | 2        | 0.22          |
| (1,1577) | 1:85:A:TYR:H     | 1:68:A:VAL:H     | 10       | 0.22          |
| (1,1563) | 1:100:A:LEU:HG   | 1:102:A:SER:H    | 9        | 0.22          |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG21  | 9        | 0.22          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 9        | 0.22          |
| (1,1516) | 1:49:A:MET:HB3   | 1:49:A:MET:H     | 1        | 0.22          |
| (1,1516) | 1:49:A:MET:HB3   | 1:49:A:MET:H     | 4        | 0.22          |
| (1,1516) | 1:49:A:MET:HB3   | 1:49:A:MET:H     | 5        | 0.22          |
| (1,1504) | 1:96:A:ALA:HB2   | 1:95:A:GLY:H     | 5        | 0.22          |
| (1,1482) | 1:131:A:VAL:HB   | 1:37:A:ILE:H     | 8        | 0.22          |
| (1,1481) | 1:37:A:ILE:HG23  | 1:131:A:VAL:HB   | 3        | 0.22          |
| (1,1481) | 1:37:A:ILE:HG23  | 1:131:A:VAL:HB   | 6        | 0.22          |
| (1,1462) | 1:45:A:SER:HB2   | 1:44:A:GLU:HB3   | 5        | 0.22          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD2   | 2        | 0.22          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD1   | 4        | 0.22          |
| (1,1432) | 1:47:A:LEU:H     | 1:57:A:TYR:HD2   | 10       | 0.22          |
| (1,1339) | 1:40:A:ILE:HG23  | 1:128:A:ASN:HD22 | 5        | 0.22          |
| (1,1332) | 1:84:A:GLY:H     | 1:67:A:LEU:HA    | 10       | 0.22          |
| (1,1279) | 1:98:A:TYR:H     | 1:64:A:LEU:HB2   | 8        | 0.22          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 3        | 0.22          |
| (1,1275) | 1:129:A:TRP:HE1  | 1:130:A:ASN:HB2  | 10       | 0.22          |
| (1,1248) | 1:57:A:TYR:H     | 1:57:A:TYR:HE1   | 7        | 0.22          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 1        | 0.22          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 4        | 0.22          |
| (1,1198) | 1:99:A:GLN:HE21  | 1:99:A:GLN:HA    | 4        | 0.22          |
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 9        | 0.22          |
| (1,966)  | 1:96:A:ALA:H     | 1:94:A:TRP:HZ3   | 7        | 0.22          |
| (1,922)  | 1:86:A:ILE:HD11  | 1:88:A:ARG:H     | 10       | 0.22          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 5        | 0.22          |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG21 | 5        | 0.22          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 5        | 0.22          |
| (1,779)  | 1:40:A:ILE:HG22  | 1:112:A:PHE:HA   | 5        | 0.22          |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2   | 8        | 0.22          |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 9        | 0.22          |
| (1,738)  | 1:78:A:ARG:HD3   | 1:54:A:ASN:H     | 3        | 0.22          |
| (1,658)  | 1:111:A:VAL:HG23 | 1:44:A:GLU:HA    | 6        | 0.22          |
| (1,658)  | 1:111:A:VAL:HG21 | 1:44:A:GLU:HA    | 7        | 0.22          |
| (1,657)  | 1:111:A:VAL:HG23 | 1:43:A:LEU:HD12  | 8        | 0.22          |
| (1,610)  | 1:66:A:ALA:HB2   | 1:62:A:GLN:HE21  | 9        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG23  | 1        | 0.22          |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG21  | 9        | 0.22          |
| (1,469)  | 1:44:A:GLU:HG3   | 1:44:A:GLU:HA    | 9        | 0.22          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 2        | 0.22          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 3        | 0.22          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 4        | 0.22          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 5        | 0.22          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 7        | 0.22          |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD21  | 7        | 0.22          |
| (1,326)  | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 8        | 0.22          |
| (1,298)  | 1:101:A:VAL:HG11 | 1:110:A:ASP:HB2  | 7        | 0.22          |
| (1,282)  | 1:78:A:ARG:HD2   | 1:78:A:ARG:HG3   | 2        | 0.22          |
| (1,282)  | 1:78:A:ARG:HD2   | 1:78:A:ARG:HG2   | 4        | 0.22          |
| (1,278)  | 1:86:A:ILE:HD13  | 1:67:A:LEU:HB3   | 1        | 0.22          |
| (1,278)  | 1:86:A:ILE:HD11  | 1:67:A:LEU:HB3   | 7        | 0.22          |
| (1,228)  | 1:63:A:GLY:HA2   | 1:100:A:LEU:HB2  | 9        | 0.22          |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 4        | 0.22          |
| (1,180)  | 1:114:A:TYR:HB2  | 1:119:A:MET:HA   | 6        | 0.22          |
| (1,134)  | 1:122:A:THR:HG23 | 1:123:A:ASP:H    | 1        | 0.22          |
| (1,57)   | 1:34:A:GLN:HA    | 1:37:A:ILE:H     | 1        | 0.22          |
| (1,57)   | 1:34:A:GLN:HA    | 1:37:A:ILE:H     | 2        | 0.22          |
| (1,1581) | 1:41:A:VAL:H     | 1:42:A:ALA:HA    | 2        | 0.21          |
| (1,1570) | 1:79:A:SER:H     | 1:53:A:ASP:HB3   | 1        | 0.21          |
| (1,1547) | 1:79:A:SER:HB2   | 1:80:A:TYR:H     | 8        | 0.21          |
| (1,1516) | 1:49:A:MET:HB3   | 1:49:A:MET:H     | 2        | 0.21          |
| (1,1494) | 1:122:A:THR:HG21 | 1:121:A:ASP:HB3  | 5        | 0.21          |
| (1,1484) | 1:64:A:LEU:HD21  | 1:63:A:GLY:HA2   | 3        | 0.21          |
| (1,1479) | 1:52:A:LEU:HG    | 1:49:A:MET:HA    | 2        | 0.21          |
| (1,1457) | 1:41:A:VAL:HB    | 1:133:A:THR:H    | 1        | 0.21          |
| (1,1411) | 1:66:A:ALA:HB2   | 1:68:A:VAL:H     | 6        | 0.21          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 10       | 0.21          |
| (1,1374) | 1:99:A:GLN:H     | 1:100:A:LEU:HB3  | 4        | 0.21          |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG11  | 1        | 0.21          |
| (1,1261) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD21 | 7        | 0.21          |
| (1,1248) | 1:57:A:TYR:H     | 1:57:A:TYR:HE1   | 2        | 0.21          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 5        | 0.21          |
| (1,1222) | 1:107:A:GLY:H    | 1:105:A:ARG:HB2  | 3        | 0.21          |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG11 | 3        | 0.21          |
| (1,1041) | 1:100:A:LEU:HB2  | 1:100:A:LEU:H    | 8        | 0.21          |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 2        | 0.21          |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 4        | 0.21          |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 6        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG2   | 7        | 0.21          |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 9        | 0.21          |
| (1,1007) | 1:109:A:VAL:H    | 1:108:A:LYS:HD3  | 8        | 0.21          |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 10       | 0.21          |
| (1,908)  | 1:117:A:ASP:HB2  | 1:117:A:ASP:H    | 7        | 0.21          |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 2        | 0.21          |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 10       | 0.21          |
| (1,838)  | 1:57:A:TYR:H     | 1:57:A:TYR:HB3   | 1        | 0.21          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 9        | 0.21          |
| (1,764)  | 1:44:A:GLU:HG2   | 1:128:A:ASN:HD21 | 8        | 0.21          |
| (1,764)  | 1:44:A:GLU:HG2   | 1:128:A:ASN:HD21 | 9        | 0.21          |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 3        | 0.21          |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 6        | 0.21          |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 10       | 0.21          |
| (1,726)  | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 10       | 0.21          |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 2        | 0.21          |
| (1,696)  | 1:100:A:LEU:HD12 | 1:100:A:LEU:HA   | 3        | 0.21          |
| (1,696)  | 1:100:A:LEU:HD11 | 1:100:A:LEU:HA   | 5        | 0.21          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 5        | 0.21          |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 8        | 0.21          |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG21 | 6        | 0.21          |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG23 | 7        | 0.21          |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG21 | 9        | 0.21          |
| (1,667)  | 1:109:A:VAL:HG21 | 1:108:A:LYS:HB2  | 8        | 0.21          |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2   | 1        | 0.21          |
| (1,658)  | 1:111:A:VAL:HG22 | 1:44:A:GLU:HA    | 2        | 0.21          |
| (1,658)  | 1:111:A:VAL:HG22 | 1:44:A:GLU:HA    | 10       | 0.21          |
| (1,648)  | 1:42:A:ALA:HA    | 1:42:A:ALA:HB1   | 8        | 0.21          |
| (1,618)  | 1:100:A:LEU:HD22 | 1:100:A:LEU:H    | 1        | 0.21          |
| (1,595)  | 1:123:A:ASP:HA   | 1:123:A:ASP:HB3  | 4        | 0.21          |
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 7        | 0.21          |
| (1,554)  | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 1        | 0.21          |
| (1,553)  | 1:85:A:TYR:HB3   | 1:85:A:TYR:H     | 6        | 0.21          |
| (1,514)  | 1:51:A:LYS:HG3   | 1:56:A:ARG:HA    | 7        | 0.21          |
| (1,474)  | 1:69:A:LYS:HB2   | 1:68:A:VAL:HB    | 1        | 0.21          |
| (1,474)  | 1:69:A:LYS:HB2   | 1:68:A:VAL:HB    | 4        | 0.21          |
| (1,470)  | 1:57:A:TYR:HB3   | 1:56:A:ARG:HD3   | 4        | 0.21          |
| (1,435)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:H     | 8        | 0.21          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 6        | 0.21          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 9        | 0.21          |
| (1,426)  | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 10       | 0.21          |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG22  | 2        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,408)  | 1:61:A:GLU:HA   | 1:60:A:THR:HG22 | 9        | 0.21          |
| (1,337)  | 1:52:A:LEU:HD12 | 1:52:A:LEU:HB3  | 2        | 0.21          |
| (1,336)  | 1:52:A:LEU:HD21 | 1:48:A:ASP:HB3  | 6        | 0.21          |
| (1,336)  | 1:52:A:LEU:HD22 | 1:48:A:ASP:HB3  | 9        | 0.21          |
| (1,255)  | 1:43:A:LEU:HB3  | 1:40:A:ILE:HA   | 10       | 0.21          |
| (1,228)  | 1:63:A:GLY:HA2  | 1:100:A:LEU:HB2 | 2        | 0.21          |
| (1,180)  | 1:114:A:TYR:HB2 | 1:119:A:MET:HA  | 2        | 0.21          |
| (1,180)  | 1:114:A:TYR:HB2 | 1:119:A:MET:HA  | 8        | 0.21          |
| (1,46)   | 1:61:A:GLU:HB3  | 1:73:A:THR:HG23 | 3        | 0.21          |
| (1,29)   | 1:105:A:ARG:HA  | 1:105:A:ARG:HB3 | 1        | 0.21          |
| (1,21)   | 1:31:A:ALA:HA   | 1:30:A:LYS:HB3  | 7        | 0.21          |
| (1,11)   | 1:69:A:LYS:HE3  | 1:69:A:LYS:HG2  | 7        | 0.21          |
| (1,1587) | 1:127:A:GLY:H   | 1:40:A:ILE:HD13 | 3        | 0.2           |
| (1,1583) | 1:50:A:TYR:H    | 1:46:A:ALA:HB2  | 4        | 0.2           |
| (1,1580) | 1:48:A:ASP:H    | 1:52:A:LEU:HD22 | 1        | 0.2           |
| (1,1580) | 1:48:A:ASP:H    | 1:52:A:LEU:HD21 | 5        | 0.2           |
| (1,1580) | 1:48:A:ASP:H    | 1:67:A:LEU:HD21 | 8        | 0.2           |
| (1,1577) | 1:85:A:TYR:H    | 1:68:A:VAL:H    | 4        | 0.2           |
| (1,1516) | 1:49:A:MET:HB3  | 1:49:A:MET:H    | 3        | 0.2           |
| (1,1516) | 1:49:A:MET:HB3  | 1:49:A:MET:H    | 6        | 0.2           |
| (1,1516) | 1:49:A:MET:HB3  | 1:49:A:MET:H    | 7        | 0.2           |
| (1,1516) | 1:49:A:MET:HB3  | 1:49:A:MET:H    | 8        | 0.2           |
| (1,1516) | 1:49:A:MET:HB3  | 1:49:A:MET:H    | 9        | 0.2           |
| (1,1500) | 1:69:A:LYS:HG2  | 1:69:A:LYS:HA   | 5        | 0.2           |
| (1,1479) | 1:52:A:LEU:HG   | 1:49:A:MET:HA   | 1        | 0.2           |
| (1,1479) | 1:52:A:LEU:HG   | 1:49:A:MET:HA   | 3        | 0.2           |
| (1,1462) | 1:45:A:SER:HB2  | 1:44:A:GLU:HB3  | 6        | 0.2           |
| (1,1457) | 1:41:A:VAL:HB   | 1:133:A:THR:H   | 3        | 0.2           |
| (1,1444) | 1:27:A:ASN:HB3  | 1:30:A:LYS:HB3  | 7        | 0.2           |
| (1,1444) | 1:27:A:ASN:HB3  | 1:28:A:LYS:HB2  | 8        | 0.2           |
| (1,1441) | 1:79:A:SER:H    | 1:85:A:TYR:HE2  | 3        | 0.2           |
| (1,1411) | 1:66:A:ALA:HB3  | 1:68:A:VAL:H    | 5        | 0.2           |
| (1,1411) | 1:66:A:ALA:HB2  | 1:68:A:VAL:H    | 7        | 0.2           |
| (1,1374) | 1:99:A:GLN:H    | 1:100:A:LEU:HB3 | 1        | 0.2           |
| (1,1332) | 1:84:A:GLY:H    | 1:67:A:LEU:HA   | 1        | 0.2           |
| (1,1301) | 1:85:A:TYR:H    | 1:85:A:TYR:HE1  | 1        | 0.2           |
| (1,1198) | 1:99:A:GLN:HE21 | 1:99:A:GLN:HA   | 5        | 0.2           |
| (1,1175) | 1:26:A:GLY:H    | 1:28:A:LYS:HA   | 2        | 0.2           |
| (1,1049) | 1:51:A:LYS:HG2  | 1:56:A:ARG:H    | 1        | 0.2           |
| (1,1041) | 1:100:A:LEU:HB2 | 1:100:A:LEU:H   | 2        | 0.2           |
| (1,1041) | 1:100:A:LEU:HB2 | 1:100:A:LEU:H   | 10       | 0.2           |
| (1,1034) | 1:91:A:GLN:HE21 | 1:91:A:GLN:HG3  | 1        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 3        | 0.2           |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 8        | 0.2           |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 10       | 0.2           |
| (1,922)  | 1:86:A:ILE:HD13  | 1:88:A:ARG:H     | 5        | 0.2           |
| (1,920)  | 1:87:A:ARG:HB2   | 1:88:A:ARG:H     | 1        | 0.2           |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG21 | 3        | 0.2           |
| (1,908)  | 1:117:A:ASP:HB2  | 1:117:A:ASP:H    | 3        | 0.2           |
| (1,908)  | 1:117:A:ASP:HB2  | 1:117:A:ASP:H    | 5        | 0.2           |
| (1,908)  | 1:117:A:ASP:HB2  | 1:117:A:ASP:H    | 6        | 0.2           |
| (1,880)  | 1:29:A:GLU:H     | 1:29:A:GLU:HG3   | 5        | 0.2           |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 6        | 0.2           |
| (1,802)  | 1:33:A:ARG:HG3   | 1:37:A:ILE:H     | 6        | 0.2           |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 1        | 0.2           |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 2        | 0.2           |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 3        | 0.2           |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 5        | 0.2           |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 8        | 0.2           |
| (1,784)  | 1:114:A:TYR:HA   | 1:126:A:ILE:HB   | 3        | 0.2           |
| (1,779)  | 1:40:A:ILE:HG21  | 1:112:A:PHE:HA   | 4        | 0.2           |
| (1,779)  | 1:40:A:ILE:HG22  | 1:112:A:PHE:HA   | 9        | 0.2           |
| (1,744)  | 1:86:A:ILE:HG13  | 1:67:A:LEU:HB3   | 4        | 0.2           |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 1        | 0.2           |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE1  | 5        | 0.2           |
| (1,741)  | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 8        | 0.2           |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 1        | 0.2           |
| (1,740)  | 1:132:A:GLY:HA3  | 1:131:A:VAL:H    | 9        | 0.2           |
| (1,738)  | 1:78:A:ARG:HD2   | 1:54:A:ASN:H     | 6        | 0.2           |
| (1,726)  | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 2        | 0.2           |
| (1,726)  | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 4        | 0.2           |
| (1,699)  | 1:101:A:VAL:HG23 | 1:105:A:ARG:HD2  | 4        | 0.2           |
| (1,696)  | 1:100:A:LEU:HD11 | 1:100:A:LEU:HA   | 6        | 0.2           |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 7        | 0.2           |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 10       | 0.2           |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 6        | 0.2           |
| (1,677)  | 1:37:A:ILE:HA    | 1:41:A:VAL:H     | 7        | 0.2           |
| (1,670)  | 1:111:A:VAL:HG12 | 1:109:A:VAL:HG23 | 2        | 0.2           |
| (1,658)  | 1:111:A:VAL:HG22 | 1:44:A:GLU:HA    | 5        | 0.2           |
| (1,657)  | 1:111:A:VAL:HG21 | 1:43:A:LEU:HD13  | 4        | 0.2           |
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 10       | 0.2           |
| (1,544)  | 1:57:A:TYR:HA    | 1:57:A:TYR:HD1   | 1        | 0.2           |
| (1,500)  | 1:71:A:PRO:HA    | 1:72:A:THR:HG23  | 5        | 0.2           |
| (1,483)  | 1:59:A:THR:HG23  | 1:58:A:PRO:HA    | 1        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,435)  | 1:41:A:VAL:HG13  | 1:42:A:ALA:H     | 7        | 0.2           |
| (1,435)  | 1:41:A:VAL:HG11  | 1:42:A:ALA:H     | 9        | 0.2           |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG21  | 1        | 0.2           |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG23  | 5        | 0.2           |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG23  | 7        | 0.2           |
| (1,408)  | 1:61:A:GLU:HA    | 1:60:A:THR:HG22  | 10       | 0.2           |
| (1,407)  | 1:61:A:GLU:HA    | 1:61:A:GLU:HG3   | 3        | 0.2           |
| (1,367)  | 1:103:A:PRO:HB3  | 1:104:A:GLY:H    | 3        | 0.2           |
| (1,337)  | 1:52:A:LEU:HD12  | 1:52:A:LEU:HB3   | 1        | 0.2           |
| (1,337)  | 1:52:A:LEU:HD11  | 1:52:A:LEU:HB3   | 3        | 0.2           |
| (1,255)  | 1:43:A:LEU:HB3   | 1:40:A:ILE:HA    | 7        | 0.2           |
| (1,151)  | 1:38:A:SER:HB2   | 1:90:A:PRO:HB3   | 6        | 0.2           |
| (1,85)   | 1:37:A:ILE:HA    | 1:40:A:ILE:HD13  | 1        | 0.2           |
| (1,85)   | 1:37:A:ILE:HA    | 1:40:A:ILE:HD11  | 7        | 0.2           |
| (1,57)   | 1:34:A:GLN:HA    | 1:37:A:ILE:H     | 4        | 0.2           |
| (1,21)   | 1:31:A:ALA:HA    | 1:30:A:LYS:HB3   | 1        | 0.2           |
| (1,21)   | 1:31:A:ALA:HA    | 1:30:A:LYS:HB3   | 5        | 0.2           |
| (1,21)   | 1:31:A:ALA:HA    | 1:30:A:LYS:HB3   | 8        | 0.2           |
| (1,12)   | 1:105:A:ARG:HD2  | 1:105:A:ARG:HA   | 4        | 0.2           |
| (1,1595) | 1:32:A:ASP:H     | 1:30:A:LYS:HB3   | 10       | 0.19          |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB2   | 2        | 0.19          |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB1   | 9        | 0.19          |
| (1,1556) | 1:56:A:ARG:H     | 1:54:A:ASN:H     | 2        | 0.19          |
| (1,1457) | 1:41:A:VAL:HB    | 1:133:A:THR:H    | 8        | 0.19          |
| (1,1411) | 1:66:A:ALA:HB2   | 1:68:A:VAL:H     | 4        | 0.19          |
| (1,1410) | 1:65:A:GLY:HA3   | 1:68:A:VAL:H     | 2        | 0.19          |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 3        | 0.19          |
| (1,1350) | 1:54:A:ASN:HB2   | 1:52:A:LEU:H     | 5        | 0.19          |
| (1,1261) | 1:109:A:VAL:HG12 | 1:128:A:ASN:HD21 | 1        | 0.19          |
| (1,1248) | 1:57:A:TYR:H     | 1:57:A:TYR:HE1   | 3        | 0.19          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 9        | 0.19          |
| (1,1080) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HB3   | 8        | 0.19          |
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 3        | 0.19          |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG13 | 2        | 0.19          |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG13 | 10       | 0.19          |
| (1,1034) | 1:91:A:GLN:HE21  | 1:91:A:GLN:HG3   | 5        | 0.19          |
| (1,966)  | 1:96:A:ALA:H     | 1:94:A:TRP:HZ3   | 8        | 0.19          |
| (1,904)  | 1:106:A:HIS:HB3  | 1:107:A:GLY:H    | 6        | 0.19          |
| (1,888)  | 1:108:A:LYS:HB3  | 1:108:A:LYS:H    | 6        | 0.19          |
| (1,827)  | 1:89:A:LEU:HB2   | 1:89:A:LEU:H     | 5        | 0.19          |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 6        | 0.19          |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 7        | 0.19          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,788) | 1:88:A:ARG:HA    | 1:87:A:ARG:H     | 9        | 0.19          |
| (1,784) | 1:114:A:TYR:HA   | 1:126:A:ILE:HB   | 9        | 0.19          |
| (1,776) | 1:73:A:THR:HB    | 1:61:A:GLU:HG2   | 6        | 0.19          |
| (1,758) | 1:49:A:MET:HG3   | 1:52:A:LEU:HD21  | 2        | 0.19          |
| (1,741) | 1:114:A:TYR:HB2  | 1:114:A:TYR:HE2  | 2        | 0.19          |
| (1,726) | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 5        | 0.19          |
| (1,720) | 1:108:A:LYS:HA   | 1:103:A:PRO:HB3  | 4        | 0.19          |
| (1,720) | 1:108:A:LYS:HA   | 1:103:A:PRO:HB3  | 9        | 0.19          |
| (1,720) | 1:108:A:LYS:HA   | 1:103:A:PRO:HB3  | 10       | 0.19          |
| (1,674) | 1:109:A:VAL:HG21 | 1:57:A:TYR:HD2   | 3        | 0.19          |
| (1,670) | 1:111:A:VAL:HG13 | 1:109:A:VAL:HG22 | 3        | 0.19          |
| (1,621) | 1:66:A:ALA:HA    | 1:69:A:LYS:HB2   | 6        | 0.19          |
| (1,610) | 1:66:A:ALA:HB3   | 1:62:A:GLN:HE21  | 6        | 0.19          |
| (1,595) | 1:123:A:ASP:HA   | 1:123:A:ASP:HB3  | 8        | 0.19          |
| (1,554) | 1:85:A:TYR:HB3   | 1:86:A:ILE:H     | 4        | 0.19          |
| (1,553) | 1:85:A:TYR:HB3   | 1:85:A:TYR:H     | 1        | 0.19          |
| (1,553) | 1:85:A:TYR:HB3   | 1:85:A:TYR:H     | 7        | 0.19          |
| (1,552) | 1:85:A:TYR:HB3   | 1:67:A:LEU:HA    | 5        | 0.19          |
| (1,534) | 1:109:A:VAL:HB   | 1:57:A:TYR:HD2   | 6        | 0.19          |
| (1,514) | 1:51:A:LYS:HG3   | 1:56:A:ARG:HA    | 4        | 0.19          |
| (1,486) | 1:75:A:PRO:HG2   | 1:59:A:THR:HG23  | 1        | 0.19          |
| (1,486) | 1:75:A:PRO:HG2   | 1:59:A:THR:HG22  | 4        | 0.19          |
| (1,486) | 1:75:A:PRO:HG2   | 1:59:A:THR:HG21  | 7        | 0.19          |
| (1,474) | 1:69:A:LYS:HB2   | 1:68:A:VAL:HB    | 7        | 0.19          |
| (1,435) | 1:41:A:VAL:HG13  | 1:42:A:ALA:H     | 4        | 0.19          |
| (1,435) | 1:41:A:VAL:HG12  | 1:42:A:ALA:H     | 10       | 0.19          |
| (1,426) | 1:75:A:PRO:HG3   | 1:75:A:PRO:HA    | 1        | 0.19          |
| (1,355) | 1:131:A:VAL:HB   | 1:131:A:VAL:H    | 8        | 0.19          |
| (1,337) | 1:52:A:LEU:HD11  | 1:52:A:LEU:HB3   | 4        | 0.19          |
| (1,318) | 1:124:A:ASP:HA   | 1:124:A:ASP:HB3  | 5        | 0.19          |
| (1,318) | 1:124:A:ASP:HA   | 1:124:A:ASP:HB3  | 10       | 0.19          |
| (1,282) | 1:78:A:ARG:HD3   | 1:78:A:ARG:HG2   | 3        | 0.19          |
| (1,282) | 1:78:A:ARG:HD2   | 1:78:A:ARG:HG3   | 6        | 0.19          |
| (1,282) | 1:78:A:ARG:HD2   | 1:78:A:ARG:HG3   | 7        | 0.19          |
| (1,282) | 1:78:A:ARG:HD3   | 1:78:A:ARG:HG2   | 9        | 0.19          |
| (1,270) | 1:85:A:TYR:HA    | 1:81:A:PRO:HB2   | 5        | 0.19          |
| (1,270) | 1:85:A:TYR:HA    | 1:81:A:PRO:HB2   | 10       | 0.19          |
| (1,255) | 1:43:A:LEU:HB3   | 1:40:A:ILE:HA    | 3        | 0.19          |
| (1,255) | 1:43:A:LEU:HB3   | 1:40:A:ILE:HA    | 6        | 0.19          |
| (1,222) | 1:88:A:ARG:HD3   | 1:88:A:ARG:HB2   | 1        | 0.19          |
| (1,165) | 1:30:A:LYS:HA    | 1:30:A:LYS:HB2   | 2        | 0.19          |
| (1,57)  | 1:34:A:GLN:HA    | 1:37:A:ILE:H     | 5        | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,43)   | 1:33:A:ARG:HB3   | 1:34:A:GLN:H    | 7        | 0.19          |
| (1,29)   | 1:105:A:ARG:HA   | 1:105:A:ARG:HB3 | 8        | 0.19          |
| (1,21)   | 1:31:A:ALA:HA    | 1:30:A:LYS:HB3  | 6        | 0.19          |
| (1,10)   | 1:28:A:LYS:HE3   | 1:28:A:LYS:HD2  | 6        | 0.19          |
| (1,10)   | 1:28:A:LYS:HE2   | 1:28:A:LYS:HD2  | 7        | 0.19          |
| (1,1595) | 1:32:A:ASP:H     | 1:30:A:LYS:HB3  | 8        | 0.18          |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB3  | 3        | 0.18          |
| (1,1562) | 1:102:A:SER:H    | 1:60:A:THR:HG21 | 8        | 0.18          |
| (1,1516) | 1:49:A:MET:HB3   | 1:49:A:MET:H    | 10       | 0.18          |
| (1,1497) | 1:73:A:THR:HB    | 1:62:A:GLN:HG2  | 8        | 0.18          |
| (1,1481) | 1:37:A:ILE:HG22  | 1:131:A:VAL:HB  | 7        | 0.18          |
| (1,1345) | 1:126:A:ILE:H    | 1:113:A:SER:HB2 | 10       | 0.18          |
| (1,1301) | 1:85:A:TYR:H     | 1:85:A:TYR:HE1  | 6        | 0.18          |
| (1,1301) | 1:85:A:TYR:H     | 1:85:A:TYR:HE2  | 7        | 0.18          |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG11 | 6        | 0.18          |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG11 | 8        | 0.18          |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG11 | 9        | 0.18          |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG12 | 10       | 0.18          |
| (1,1269) | 1:55:A:SER:H     | 1:51:A:LYS:HD3  | 10       | 0.18          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2 | 7        | 0.18          |
| (1,1187) | 1:62:A:GLN:HE22  | 1:62:A:GLN:HB3  | 1        | 0.18          |
| (1,1177) | 1:27:A:ASN:H     | 1:24:A:GLY:HA2  | 2        | 0.18          |
| (1,1082) | 1:62:A:GLN:HE21  | 1:71:A:PRO:HG2  | 10       | 0.18          |
| (1,1041) | 1:100:A:LEU:HB2  | 1:100:A:LEU:H   | 3        | 0.18          |
| (1,984)  | 1:96:A:ALA:HB3   | 1:97:A:GLU:H    | 9        | 0.18          |
| (1,927)  | 1:49:A:MET:HB3   | 1:49:A:MET:H    | 1        | 0.18          |
| (1,927)  | 1:49:A:MET:HB3   | 1:49:A:MET:H    | 4        | 0.18          |
| (1,927)  | 1:49:A:MET:HB3   | 1:49:A:MET:H    | 5        | 0.18          |
| (1,922)  | 1:86:A:ILE:HD12  | 1:88:A:ARG:H    | 7        | 0.18          |
| (1,904)  | 1:106:A:HIS:HB3  | 1:107:A:GLY:H   | 1        | 0.18          |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG21 | 1        | 0.18          |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG22 | 2        | 0.18          |
| (1,852)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:H   | 9        | 0.18          |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H    | 4        | 0.18          |
| (1,788)  | 1:88:A:ARG:HA    | 1:87:A:ARG:H    | 10       | 0.18          |
| (1,784)  | 1:114:A:TYR:HA   | 1:126:A:ILE:HB  | 2        | 0.18          |
| (1,783)  | 1:125:A:ASP:HA   | 1:126:A:ILE:HB  | 10       | 0.18          |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2  | 2        | 0.18          |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2  | 3        | 0.18          |
| (1,770)  | 1:118:A:GLY:HA3  | 1:114:A:TYR:HD2 | 6        | 0.18          |
| (1,767)  | 1:122:A:THR:HG21 | 1:121:A:ASP:H   | 2        | 0.18          |
| (1,767)  | 1:122:A:THR:HG23 | 1:121:A:ASP:H   | 6        | 0.18          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,745) | 1:140:A:SER:HB3 | 1:138:A:ASN:HD22 | 4        | 0.18          |
| (1,742) | 1:31:A:ALA:HA   | 1:33:A:ARG:HG2   | 2        | 0.18          |
| (1,742) | 1:31:A:ALA:HA   | 1:33:A:ARG:HG2   | 3        | 0.18          |
| (1,741) | 1:114:A:TYR:HB2 | 1:114:A:TYR:HE2  | 4        | 0.18          |
| (1,738) | 1:78:A:ARG:HD3  | 1:54:A:ASN:H     | 8        | 0.18          |
| (1,726) | 1:101:A:VAL:HB  | 1:100:A:LEU:HA   | 1        | 0.18          |
| (1,720) | 1:108:A:LYS:HA  | 1:103:A:PRO:HB3  | 8        | 0.18          |
| (1,663) | 1:85:A:TYR:HA   | 1:85:A:TYR:HD2   | 7        | 0.18          |
| (1,663) | 1:85:A:TYR:HA   | 1:85:A:TYR:HD2   | 10       | 0.18          |
| (1,614) | 1:60:A:THR:HA   | 1:100:A:LEU:HD22 | 6        | 0.18          |
| (1,610) | 1:66:A:ALA:HB3  | 1:62:A:GLN:HE21  | 2        | 0.18          |
| (1,595) | 1:123:A:ASP:HA  | 1:123:A:ASP:HB3  | 5        | 0.18          |
| (1,552) | 1:85:A:TYR:HB3  | 1:67:A:LEU:HA    | 2        | 0.18          |
| (1,552) | 1:85:A:TYR:HB3  | 1:67:A:LEU:HA    | 10       | 0.18          |
| (1,544) | 1:57:A:TYR:HA   | 1:57:A:TYR:HD2   | 8        | 0.18          |
| (1,514) | 1:51:A:LYS:HG3  | 1:56:A:ARG:HA    | 9        | 0.18          |
| (1,486) | 1:75:A:PRO:HG2  | 1:59:A:THR:HG21  | 10       | 0.18          |
| (1,483) | 1:59:A:THR:HG22 | 1:58:A:PRO:HA    | 4        | 0.18          |
| (1,466) | 1:82:A:GLN:HG3  | 1:83:A:ASP:H     | 3        | 0.18          |
| (1,435) | 1:41:A:VAL:HG11 | 1:42:A:ALA:H     | 6        | 0.18          |
| (1,408) | 1:61:A:GLU:HA   | 1:60:A:THR:HG23  | 3        | 0.18          |
| (1,408) | 1:61:A:GLU:HA   | 1:60:A:THR:HG22  | 4        | 0.18          |
| (1,408) | 1:61:A:GLU:HA   | 1:60:A:THR:HG21  | 6        | 0.18          |
| (1,387) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H     | 6        | 0.18          |
| (1,367) | 1:103:A:PRO:HB3 | 1:104:A:GLY:H    | 8        | 0.18          |
| (1,367) | 1:103:A:PRO:HB3 | 1:104:A:GLY:H    | 9        | 0.18          |
| (1,355) | 1:131:A:VAL:HB  | 1:131:A:VAL:H    | 1        | 0.18          |
| (1,355) | 1:131:A:VAL:HB  | 1:131:A:VAL:H    | 4        | 0.18          |
| (1,350) | 1:112:A:PHE:HA  | 1:112:A:PHE:HD1  | 3        | 0.18          |
| (1,350) | 1:112:A:PHE:HA  | 1:112:A:PHE:HD2  | 9        | 0.18          |
| (1,318) | 1:124:A:ASP:HA  | 1:124:A:ASP:HB3  | 1        | 0.18          |
| (1,318) | 1:124:A:ASP:HA  | 1:124:A:ASP:HB3  | 4        | 0.18          |
| (1,318) | 1:124:A:ASP:HA  | 1:124:A:ASP:HB3  | 7        | 0.18          |
| (1,318) | 1:124:A:ASP:HA  | 1:124:A:ASP:HB3  | 9        | 0.18          |
| (1,270) | 1:85:A:TYR:HA   | 1:81:A:PRO:HB2   | 4        | 0.18          |
| (1,255) | 1:43:A:LEU:HB3  | 1:40:A:ILE:HA    | 4        | 0.18          |
| (1,255) | 1:43:A:LEU:HB3  | 1:40:A:ILE:HA    | 5        | 0.18          |
| (1,228) | 1:63:A:GLY:HA2  | 1:100:A:LEU:HB2  | 6        | 0.18          |
| (1,222) | 1:88:A:ARG:HD3  | 1:88:A:ARG:HB2   | 7        | 0.18          |
| (1,163) | 1:88:A:ARG:HB3  | 1:88:A:ARG:H     | 6        | 0.18          |
| (1,128) | 1:41:A:VAL:HA   | 1:44:A:GLU:HB3   | 2        | 0.18          |
| (1,85)  | 1:37:A:ILE:HA   | 1:40:A:ILE:HD13  | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,85)   | 1:37:A:ILE:HA   | 1:40:A:ILE:HD13  | 8        | 0.18          |
| (1,54)   | 1:28:A:LYS:HD3  | 1:28:A:LYS:HG2   | 7        | 0.18          |
| (1,54)   | 1:28:A:LYS:HD2  | 1:28:A:LYS:HG2   | 9        | 0.18          |
| (1,21)   | 1:31:A:ALA:HA   | 1:30:A:LYS:HB3   | 9        | 0.18          |
| (1,12)   | 1:105:A:ARG:HD3 | 1:105:A:ARG:HA   | 5        | 0.18          |
| (1,11)   | 1:69:A:LYS:HE2  | 1:69:A:LYS:HG3   | 5        | 0.18          |
| (1,10)   | 1:28:A:LYS:HE3  | 1:28:A:LYS:HD2   | 8        | 0.18          |
| (1,10)   | 1:28:A:LYS:HE2  | 1:28:A:LYS:HD3   | 9        | 0.18          |
| (1,1577) | 1:85:A:TYR:H    | 1:68:A:VAL:H     | 5        | 0.17          |
| (1,1577) | 1:85:A:TYR:H    | 1:68:A:VAL:H     | 6        | 0.17          |
| (1,1569) | 1:92:A:ASP:H    | 1:95:A:GLY:H     | 1        | 0.17          |
| (1,1563) | 1:100:A:LEU:HG  | 1:102:A:SER:H    | 1        | 0.17          |
| (1,1563) | 1:100:A:LEU:HG  | 1:102:A:SER:H    | 7        | 0.17          |
| (1,1562) | 1:102:A:SER:H   | 1:60:A:THR:HG23  | 1        | 0.17          |
| (1,1548) | 1:80:A:TYR:H    | 1:77:A:PRO:HB2   | 7        | 0.17          |
| (1,1508) | 1:66:A:ALA:HA   | 1:69:A:LYS:H     | 1        | 0.17          |
| (1,1507) | 1:58:A:PRO:HB2  | 1:100:A:LEU:HD23 | 10       | 0.17          |
| (1,1502) | 1:57:A:TYR:HA   | 1:57:A:TYR:HD1   | 5        | 0.17          |
| (1,1479) | 1:52:A:LEU:HG   | 1:49:A:MET:HA    | 8        | 0.17          |
| (1,1452) | 1:37:A:ILE:HA   | 1:37:A:ILE:HD11  | 3        | 0.17          |
| (1,1439) | 1:79:A:SER:H    | 1:78:A:ARG:HD3   | 10       | 0.17          |
| (1,1432) | 1:47:A:LEU:H    | 1:57:A:TYR:HD2   | 8        | 0.17          |
| (1,1411) | 1:66:A:ALA:HB3  | 1:68:A:VAL:H     | 1        | 0.17          |
| (1,1385) | 1:36:A:ALA:H    | 1:35:A:LYS:HG3   | 8        | 0.17          |
| (1,1380) | 1:132:A:GLY:HA2 | 1:40:A:ILE:H     | 1        | 0.17          |
| (1,1339) | 1:40:A:ILE:HG22 | 1:128:A:ASN:HD22 | 1        | 0.17          |
| (1,1294) | 1:43:A:LEU:H    | 1:41:A:VAL:HG13  | 7        | 0.17          |
| (1,1224) | 1:122:A:THR:H   | 1:120:A:PRO:HB2  | 8        | 0.17          |
| (1,1176) | 1:26:A:GLY:H    | 1:24:A:GLY:HA3   | 7        | 0.17          |
| (1,1175) | 1:26:A:GLY:H    | 1:28:A:LYS:HA    | 7        | 0.17          |
| (1,1110) | 1:36:A:ALA:H    | 1:35:A:LYS:HD2   | 8        | 0.17          |
| (1,1091) | 1:32:A:ASP:H    | 1:28:A:LYS:HG3   | 4        | 0.17          |
| (1,1043) | 1:100:A:LEU:H   | 1:111:A:VAL:HG12 | 1        | 0.17          |
| (1,1043) | 1:100:A:LEU:H   | 1:111:A:VAL:HG13 | 4        | 0.17          |
| (1,1041) | 1:100:A:LEU:HB2 | 1:100:A:LEU:H    | 9        | 0.17          |
| (1,1007) | 1:109:A:VAL:H   | 1:108:A:LYS:HD2  | 10       | 0.17          |
| (1,966)  | 1:96:A:ALA:H    | 1:94:A:TRP:HZ3   | 3        | 0.17          |
| (1,927)  | 1:49:A:MET:HB3  | 1:49:A:MET:H     | 2        | 0.17          |
| (1,908)  | 1:117:A:ASP:HB2 | 1:117:A:ASP:H    | 1        | 0.17          |
| (1,908)  | 1:117:A:ASP:HB2 | 1:117:A:ASP:H    | 10       | 0.17          |
| (1,906)  | 1:107:A:GLY:H   | 1:105:A:ARG:H    | 6        | 0.17          |
| (1,904)  | 1:106:A:HIS:HB3 | 1:107:A:GLY:H    | 3        | 0.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,904) | 1:106:A:HIS:HB3  | 1:107:A:GLY:H    | 7        | 0.17          |
| (1,867) | 1:62:A:GLN:HE22  | 1:71:A:PRO:HG3   | 3        | 0.17          |
| (1,822) | 1:76:A:GLU:HB3   | 1:76:A:GLU:H     | 8        | 0.17          |
| (1,784) | 1:114:A:TYR:HA   | 1:126:A:ILE:HB   | 4        | 0.17          |
| (1,784) | 1:114:A:TYR:HA   | 1:126:A:ILE:HB   | 5        | 0.17          |
| (1,779) | 1:40:A:ILE:HG21  | 1:112:A:PHE:HA   | 1        | 0.17          |
| (1,751) | 1:106:A:HIS:HB2  | 1:129:A:TRP:HA   | 6        | 0.17          |
| (1,726) | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 3        | 0.17          |
| (1,726) | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 6        | 0.17          |
| (1,726) | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 7        | 0.17          |
| (1,726) | 1:101:A:VAL:HB   | 1:100:A:LEU:HA   | 8        | 0.17          |
| (1,657) | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD12  | 9        | 0.17          |
| (1,614) | 1:60:A:THR:HA    | 1:100:A:LEU:HD21 | 2        | 0.17          |
| (1,584) | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 2        | 0.17          |
| (1,584) | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 6        | 0.17          |
| (1,525) | 1:61:A:GLU:HG2   | 1:73:A:THR:HG22  | 10       | 0.17          |
| (1,514) | 1:51:A:LYS:HG3   | 1:56:A:ARG:HA    | 6        | 0.17          |
| (1,483) | 1:59:A:THR:HG22  | 1:58:A:PRO:HA    | 6        | 0.17          |
| (1,483) | 1:59:A:THR:HG21  | 1:58:A:PRO:HA    | 10       | 0.17          |
| (1,435) | 1:41:A:VAL:HG13  | 1:42:A:ALA:H     | 2        | 0.17          |
| (1,435) | 1:41:A:VAL:HG11  | 1:42:A:ALA:H     | 3        | 0.17          |
| (1,387) | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 2        | 0.17          |
| (1,387) | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 4        | 0.17          |
| (1,387) | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 8        | 0.17          |
| (1,357) | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD21  | 6        | 0.17          |
| (1,355) | 1:131:A:VAL:HB   | 1:131:A:VAL:H    | 2        | 0.17          |
| (1,355) | 1:131:A:VAL:HB   | 1:131:A:VAL:H    | 3        | 0.17          |
| (1,355) | 1:131:A:VAL:HB   | 1:131:A:VAL:H    | 5        | 0.17          |
| (1,355) | 1:131:A:VAL:HB   | 1:131:A:VAL:H    | 6        | 0.17          |
| (1,355) | 1:131:A:VAL:HB   | 1:131:A:VAL:H    | 7        | 0.17          |
| (1,355) | 1:131:A:VAL:HB   | 1:131:A:VAL:H    | 9        | 0.17          |
| (1,350) | 1:112:A:PHE:HA   | 1:112:A:PHE:HD2  | 8        | 0.17          |
| (1,337) | 1:52:A:LEU:HD11  | 1:52:A:LEU:HB3   | 5        | 0.17          |
| (1,318) | 1:124:A:ASP:HA   | 1:124:A:ASP:HB3  | 6        | 0.17          |
| (1,300) | 1:73:A:THR:HG23  | 1:71:A:PRO:HB3   | 6        | 0.17          |
| (1,291) | 1:58:A:PRO:HA    | 1:62:A:GLN:HB2   | 8        | 0.17          |
| (1,282) | 1:78:A:ARG:HD3   | 1:78:A:ARG:HG2   | 8        | 0.17          |
| (1,278) | 1:86:A:ILE:HD13  | 1:67:A:LEU:HB3   | 9        | 0.17          |
| (1,270) | 1:85:A:TYR:HA    | 1:81:A:PRO:HB2   | 3        | 0.17          |
| (1,261) | 1:86:A:ILE:HG23  | 1:85:A:TYR:HB3   | 9        | 0.17          |
| (1,255) | 1:43:A:LEU:HB3   | 1:40:A:ILE:HA    | 2        | 0.17          |
| (1,255) | 1:43:A:LEU:HB3   | 1:40:A:ILE:HA    | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,255)  | 1:43:A:LEU:HB3  | 1:40:A:ILE:HA    | 9        | 0.17          |
| (1,228)  | 1:63:A:GLY:HA2  | 1:100:A:LEU:HB2  | 4        | 0.17          |
| (1,228)  | 1:63:A:GLY:HA2  | 1:100:A:LEU:HB2  | 7        | 0.17          |
| (1,222)  | 1:88:A:ARG:HD3  | 1:88:A:ARG:HB2   | 2        | 0.17          |
| (1,222)  | 1:88:A:ARG:HD3  | 1:88:A:ARG:HB2   | 3        | 0.17          |
| (1,217)  | 1:83:A:ASP:HB2  | 1:83:A:ASP:HA    | 8        | 0.17          |
| (1,165)  | 1:30:A:LYS:HA   | 1:30:A:LYS:HB2   | 8        | 0.17          |
| (1,128)  | 1:41:A:VAL:HA   | 1:44:A:GLU:HB3   | 5        | 0.17          |
| (1,85)   | 1:37:A:ILE:HA   | 1:40:A:ILE:HD13  | 3        | 0.17          |
| (1,85)   | 1:37:A:ILE:HA   | 1:40:A:ILE:HD12  | 5        | 0.17          |
| (1,85)   | 1:37:A:ILE:HA   | 1:40:A:ILE:HD11  | 9        | 0.17          |
| (1,75)   | 1:35:A:LYS:HG3  | 1:35:A:LYS:HD2   | 5        | 0.17          |
| (1,57)   | 1:34:A:GLN:HA   | 1:37:A:ILE:H     | 9        | 0.17          |
| (1,57)   | 1:34:A:GLN:HA   | 1:37:A:ILE:H     | 10       | 0.17          |
| (1,46)   | 1:61:A:GLU:HB3  | 1:73:A:THR:HG23  | 1        | 0.17          |
| (1,21)   | 1:31:A:ALA:HA   | 1:30:A:LYS:HB3   | 3        | 0.17          |
| (1,10)   | 1:28:A:LYS:HE2  | 1:28:A:LYS:HD3   | 5        | 0.17          |
| (1,1577) | 1:85:A:TYR:H    | 1:68:A:VAL:H     | 1        | 0.16          |
| (1,1569) | 1:92:A:ASP:H    | 1:95:A:GLY:H     | 8        | 0.16          |
| (1,1563) | 1:100:A:LEU:HG  | 1:102:A:SER:H    | 6        | 0.16          |
| (1,1508) | 1:66:A:ALA:HA   | 1:69:A:LYS:H     | 3        | 0.16          |
| (1,1470) | 1:86:A:ILE:HG23 | 1:85:A:TYR:H     | 10       | 0.16          |
| (1,1462) | 1:45:A:SER:HB2  | 1:44:A:GLU:HB3   | 7        | 0.16          |
| (1,1441) | 1:79:A:SER:H    | 1:85:A:TYR:HE2   | 8        | 0.16          |
| (1,1411) | 1:66:A:ALA:HB2  | 1:68:A:VAL:H     | 2        | 0.16          |
| (1,1411) | 1:66:A:ALA:HB1  | 1:68:A:VAL:H     | 8        | 0.16          |
| (1,1332) | 1:84:A:GLY:H    | 1:67:A:LEU:HA    | 4        | 0.16          |
| (1,1294) | 1:43:A:LEU:H    | 1:41:A:VAL:HG13  | 2        | 0.16          |
| (1,1294) | 1:43:A:LEU:H    | 1:41:A:VAL:HG11  | 3        | 0.16          |
| (1,1248) | 1:57:A:TYR:H    | 1:57:A:TYR:HE2   | 5        | 0.16          |
| (1,1248) | 1:57:A:TYR:H    | 1:57:A:TYR:HE2   | 9        | 0.16          |
| (1,1175) | 1:26:A:GLY:H    | 1:28:A:LYS:HA    | 8        | 0.16          |
| (1,1043) | 1:100:A:LEU:H   | 1:111:A:VAL:HG13 | 9        | 0.16          |
| (1,1041) | 1:100:A:LEU:HB2 | 1:100:A:LEU:H    | 4        | 0.16          |
| (1,1041) | 1:100:A:LEU:HB2 | 1:100:A:LEU:H    | 5        | 0.16          |
| (1,984)  | 1:96:A:ALA:HB3  | 1:97:A:GLU:H     | 3        | 0.16          |
| (1,984)  | 1:96:A:ALA:HB1  | 1:97:A:GLU:H     | 4        | 0.16          |
| (1,966)  | 1:96:A:ALA:H    | 1:94:A:TRP:HZ3   | 5        | 0.16          |
| (1,966)  | 1:96:A:ALA:H    | 1:94:A:TRP:HZ3   | 6        | 0.16          |
| (1,927)  | 1:49:A:MET:HB3  | 1:49:A:MET:H     | 3        | 0.16          |
| (1,927)  | 1:49:A:MET:HB3  | 1:49:A:MET:H     | 6        | 0.16          |
| (1,927)  | 1:49:A:MET:HB3  | 1:49:A:MET:H     | 7        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,927)  | 1:49:A:MET:HB3   | 1:49:A:MET:H     | 8        | 0.16          |
| (1,927)  | 1:49:A:MET:HB3   | 1:49:A:MET:H     | 9        | 0.16          |
| (1,904)  | 1:106:A:HIS:HB3  | 1:107:A:GLY:H    | 9        | 0.16          |
| (1,822)  | 1:76:A:GLU:HB3   | 1:76:A:GLU:H     | 6        | 0.16          |
| (1,808)  | 1:37:A:ILE:HA    | 1:132:A:GLY:HA2  | 8        | 0.16          |
| (1,803)  | 1:46:A:ALA:HB1   | 1:67:A:LEU:HA    | 9        | 0.16          |
| (1,784)  | 1:114:A:TYR:HA   | 1:126:A:ILE:HB   | 7        | 0.16          |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 8        | 0.16          |
| (1,667)  | 1:109:A:VAL:HG23 | 1:108:A:LYS:HB2  | 10       | 0.16          |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD1   | 5        | 0.16          |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2   | 9        | 0.16          |
| (1,657)  | 1:111:A:VAL:HG21 | 1:43:A:LEU:HD13  | 7        | 0.16          |
| (1,614)  | 1:60:A:THR:HA    | 1:100:A:LEU:HD23 | 7        | 0.16          |
| (1,610)  | 1:66:A:ALA:HB2   | 1:62:A:GLN:HE21  | 8        | 0.16          |
| (1,595)  | 1:123:A:ASP:HA   | 1:123:A:ASP:HB3  | 2        | 0.16          |
| (1,592)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HA    | 3        | 0.16          |
| (1,592)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HA    | 7        | 0.16          |
| (1,592)  | 1:88:A:ARG:HD2   | 1:88:A:ARG:HA    | 9        | 0.16          |
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG22  | 9        | 0.16          |
| (1,466)  | 1:82:A:GLN:HG2   | 1:83:A:ASP:H     | 9        | 0.16          |
| (1,420)  | 1:48:A:ASP:HA    | 1:57:A:TYR:HE1   | 9        | 0.16          |
| (1,387)  | 1:67:A:LEU:HB3   | 1:67:A:LEU:H     | 3        | 0.16          |
| (1,373)  | 1:110:A:ASP:HB3  | 1:101:A:VAL:HG21 | 4        | 0.16          |
| (1,300)  | 1:73:A:THR:HG23  | 1:71:A:PRO:HB3   | 5        | 0.16          |
| (1,300)  | 1:73:A:THR:HG23  | 1:71:A:PRO:HB3   | 8        | 0.16          |
| (1,291)  | 1:58:A:PRO:HA    | 1:62:A:GLN:HB2   | 5        | 0.16          |
| (1,270)  | 1:85:A:TYR:HA    | 1:81:A:PRO:HB2   | 1        | 0.16          |
| (1,270)  | 1:85:A:TYR:HA    | 1:81:A:PRO:HB2   | 2        | 0.16          |
| (1,228)  | 1:63:A:GLY:HA2   | 1:100:A:LEU:HB2  | 8        | 0.16          |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG23  | 6        | 0.16          |
| (1,136)  | 1:50:A:TYR:HA    | 1:54:A:ASN:HB2   | 9        | 0.16          |
| (1,133)  | 1:41:A:VAL:HG22  | 1:41:A:VAL:H     | 2        | 0.16          |
| (1,85)   | 1:37:A:ILE:HA    | 1:40:A:ILE:HD11  | 4        | 0.16          |
| (1,75)   | 1:35:A:LYS:HG3   | 1:35:A:LYS:HD2   | 3        | 0.16          |
| (1,54)   | 1:28:A:LYS:HD2   | 1:28:A:LYS:HG3   | 5        | 0.16          |
| (1,46)   | 1:61:A:GLU:HB3   | 1:73:A:THR:HG21  | 2        | 0.16          |
| (1,11)   | 1:69:A:LYS:HE2   | 1:69:A:LYS:HG3   | 4        | 0.16          |
| (1,11)   | 1:69:A:LYS:HE3   | 1:69:A:LYS:HG2   | 8        | 0.16          |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG12 | 3        | 0.16          |
| (1,1583) | 1:50:A:TYR:H     | 1:46:A:ALA:HB1   | 7        | 0.15          |
| (1,1577) | 1:85:A:TYR:H     | 1:68:A:VAL:H     | 8        | 0.15          |
| (1,1569) | 1:92:A:ASP:H     | 1:95:A:GLY:H     | 3        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1569) | 1:92:A:ASP:H     | 1:95:A:GLY:H     | 6        | 0.15          |
| (1,1518) | 1:30:A:LYS:HA    | 1:34:A:GLN:HG2   | 3        | 0.15          |
| (1,1507) | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD23 | 2        | 0.15          |
| (1,1502) | 1:57:A:TYR:HA    | 1:57:A:TYR:HD1   | 9        | 0.15          |
| (1,1484) | 1:64:A:LEU:HD22  | 1:63:A:GLY:HA2   | 9        | 0.15          |
| (1,1452) | 1:37:A:ILE:HA    | 1:37:A:ILE:HD12  | 6        | 0.15          |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE1   | 6        | 0.15          |
| (1,1411) | 1:66:A:ALA:HB1   | 1:68:A:VAL:H     | 9        | 0.15          |
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG3   | 7        | 0.15          |
| (1,1350) | 1:54:A:ASN:HB3   | 1:52:A:LEU:H     | 9        | 0.15          |
| (1,1345) | 1:126:A:ILE:H    | 1:113:A:SER:HB2  | 1        | 0.15          |
| (1,1345) | 1:126:A:ILE:H    | 1:113:A:SER:HB2  | 9        | 0.15          |
| (1,1294) | 1:43:A:LEU:H     | 1:41:A:VAL:HG13  | 4        | 0.15          |
| (1,1248) | 1:57:A:TYR:H     | 1:57:A:TYR:HE2   | 1        | 0.15          |
| (1,1248) | 1:57:A:TYR:H     | 1:57:A:TYR:HE1   | 6        | 0.15          |
| (1,1218) | 1:115:A:GLY:H    | 1:114:A:TYR:HB3  | 6        | 0.15          |
| (1,1175) | 1:26:A:GLY:H     | 1:28:A:LYS:HA    | 10       | 0.15          |
| (1,1053) | 1:53:A:ASP:HB3   | 1:54:A:ASN:H     | 3        | 0.15          |
| (1,1053) | 1:53:A:ASP:HB3   | 1:54:A:ASN:H     | 8        | 0.15          |
| (1,1053) | 1:53:A:ASP:HB3   | 1:54:A:ASN:H     | 9        | 0.15          |
| (1,1047) | 1:56:A:ARG:H     | 1:56:A:ARG:HG3   | 2        | 0.15          |
| (1,987)  | 1:117:A:ASP:H    | 1:119:A:MET:H    | 4        | 0.15          |
| (1,984)  | 1:96:A:ALA:HB2   | 1:97:A:GLU:H     | 6        | 0.15          |
| (1,984)  | 1:96:A:ALA:HB2   | 1:97:A:GLU:H     | 10       | 0.15          |
| (1,966)  | 1:96:A:ALA:H     | 1:94:A:TRP:HZ3   | 1        | 0.15          |
| (1,922)  | 1:86:A:ILE:HD13  | 1:88:A:ARG:H     | 4        | 0.15          |
| (1,908)  | 1:117:A:ASP:HB2  | 1:117:A:ASP:H    | 4        | 0.15          |
| (1,908)  | 1:117:A:ASP:HB2  | 1:117:A:ASP:H    | 9        | 0.15          |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG23  | 5        | 0.15          |
| (1,852)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:H    | 7        | 0.15          |
| (1,847)  | 1:70:A:LYS:H     | 1:70:A:LYS:HE3   | 5        | 0.15          |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2   | 10       | 0.15          |
| (1,750)  | 1:53:A:ASP:HB2   | 1:85:A:TYR:HD1   | 7        | 0.15          |
| (1,704)  | 1:104:A:GLY:HA3  | 1:106:A:HIS:H    | 9        | 0.15          |
| (1,696)  | 1:100:A:LEU:HD13 | 1:100:A:LEU:HA   | 9        | 0.15          |
| (1,674)  | 1:109:A:VAL:HG23 | 1:57:A:TYR:HD2   | 6        | 0.15          |
| (1,595)  | 1:123:A:ASP:HA   | 1:123:A:ASP:HB3  | 10       | 0.15          |
| (1,592)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HA    | 2        | 0.15          |
| (1,553)  | 1:85:A:TYR:HB3   | 1:85:A:TYR:H     | 8        | 0.15          |
| (1,552)  | 1:85:A:TYR:HB3   | 1:67:A:LEU:HA    | 3        | 0.15          |
| (1,552)  | 1:85:A:TYR:HB3   | 1:67:A:LEU:HA    | 4        | 0.15          |
| (1,534)  | 1:109:A:VAL:HB   | 1:57:A:TYR:HD2   | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,483)  | 1:59:A:THR:HG21 | 1:58:A:PRO:HA    | 3        | 0.15          |
| (1,483)  | 1:59:A:THR:HG23 | 1:58:A:PRO:HA    | 5        | 0.15          |
| (1,483)  | 1:59:A:THR:HG22 | 1:58:A:PRO:HA    | 9        | 0.15          |
| (1,474)  | 1:69:A:LYS:HB2  | 1:68:A:VAL:HB    | 3        | 0.15          |
| (1,474)  | 1:69:A:LYS:HB2  | 1:68:A:VAL:HB    | 6        | 0.15          |
| (1,466)  | 1:82:A:GLN:HG3  | 1:83:A:ASP:H     | 2        | 0.15          |
| (1,424)  | 1:49:A:MET:HG3  | 1:49:A:MET:H     | 10       | 0.15          |
| (1,357)  | 1:64:A:LEU:HB2  | 1:64:A:LEU:HD23  | 8        | 0.15          |
| (1,337)  | 1:52:A:LEU:HD11 | 1:52:A:LEU:HB3   | 8        | 0.15          |
| (1,318)  | 1:124:A:ASP:HA  | 1:124:A:ASP:HB3  | 3        | 0.15          |
| (1,291)  | 1:58:A:PRO:HA   | 1:62:A:GLN:HB2   | 1        | 0.15          |
| (1,291)  | 1:58:A:PRO:HA   | 1:62:A:GLN:HB2   | 4        | 0.15          |
| (1,291)  | 1:58:A:PRO:HA   | 1:62:A:GLN:HB2   | 6        | 0.15          |
| (1,291)  | 1:58:A:PRO:HA   | 1:62:A:GLN:HB2   | 10       | 0.15          |
| (1,270)  | 1:85:A:TYR:HA   | 1:81:A:PRO:HB2   | 7        | 0.15          |
| (1,270)  | 1:85:A:TYR:HA   | 1:81:A:PRO:HB2   | 8        | 0.15          |
| (1,165)  | 1:30:A:LYS:HA   | 1:30:A:LYS:HB2   | 6        | 0.15          |
| (1,165)  | 1:30:A:LYS:HA   | 1:30:A:LYS:HB2   | 7        | 0.15          |
| (1,165)  | 1:30:A:LYS:HA   | 1:30:A:LYS:HB2   | 10       | 0.15          |
| (1,163)  | 1:88:A:ARG:HB3  | 1:88:A:ARG:H     | 9        | 0.15          |
| (1,143)  | 1:133:A:THR:HB  | 1:134:A:SER:H    | 6        | 0.15          |
| (1,136)  | 1:50:A:TYR:HA   | 1:54:A:ASN:HB2   | 5        | 0.15          |
| (1,136)  | 1:50:A:TYR:HA   | 1:54:A:ASN:HB3   | 8        | 0.15          |
| (1,133)  | 1:41:A:VAL:HG21 | 1:41:A:VAL:H     | 5        | 0.15          |
| (1,128)  | 1:41:A:VAL:HA   | 1:44:A:GLU:HB3   | 6        | 0.15          |
| (1,85)   | 1:37:A:ILE:HA   | 1:40:A:ILE:HD12  | 6        | 0.15          |
| (1,75)   | 1:35:A:LYS:HG3  | 1:35:A:LYS:HD2   | 4        | 0.15          |
| (1,75)   | 1:35:A:LYS:HG3  | 1:35:A:LYS:HD2   | 7        | 0.15          |
| (1,75)   | 1:35:A:LYS:HG2  | 1:35:A:LYS:HD3   | 8        | 0.15          |
| (1,54)   | 1:28:A:LYS:HD2  | 1:28:A:LYS:HG3   | 6        | 0.15          |
| (1,17)   | 1:29:A:GLU:HG3  | 1:29:A:GLU:HA    | 7        | 0.15          |
| (1,10)   | 1:28:A:LYS:HE2  | 1:28:A:LYS:HD3   | 2        | 0.15          |
| (1,6)    | 1:130:A:ASN:HB2 | 1:131:A:VAL:HG13 | 9        | 0.15          |
| (1,1576) | 1:83:A:ASP:H    | 1:84:A:GLY:HA3   | 9        | 0.14          |
| (1,1575) | 1:118:A:GLY:H   | 1:114:A:TYR:HD2  | 1        | 0.14          |
| (1,1523) | 1:140:A:SER:HB2 | 1:139:A:GLY:H    | 10       | 0.14          |
| (1,1508) | 1:66:A:ALA:HA   | 1:69:A:LYS:H     | 9        | 0.14          |
| (1,1507) | 1:58:A:PRO:HB2  | 1:100:A:LEU:HD21 | 9        | 0.14          |
| (1,1504) | 1:96:A:ALA:HB3  | 1:95:A:GLY:H     | 1        | 0.14          |
| (1,1479) | 1:52:A:LEU:HG   | 1:49:A:MET:HA    | 4        | 0.14          |
| (1,1479) | 1:52:A:LEU:HG   | 1:49:A:MET:HA    | 7        | 0.14          |
| (1,1459) | 1:86:A:ILE:HB   | 1:86:A:ILE:HG22  | 7        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1398) | 1:51:A:LYS:H    | 1:57:A:TYR:HD2   | 3        | 0.14          |
| (1,1380) | 1:132:A:GLY:HA2 | 1:40:A:ILE:H     | 2        | 0.14          |
| (1,1380) | 1:132:A:GLY:HA2 | 1:40:A:ILE:H     | 6        | 0.14          |
| (1,1294) | 1:43:A:LEU:H    | 1:41:A:VAL:HG13  | 5        | 0.14          |
| (1,1262) | 1:134:A:SER:H   | 1:132:A:GLY:HA3  | 2        | 0.14          |
| (1,1218) | 1:115:A:GLY:H   | 1:114:A:TYR:HB3  | 7        | 0.14          |
| (1,1053) | 1:53:A:ASP:HB3  | 1:54:A:ASN:H     | 4        | 0.14          |
| (1,1015) | 1:104:A:GLY:H   | 1:110:A:ASP:H    | 3        | 0.14          |
| (1,1015) | 1:104:A:GLY:H   | 1:110:A:ASP:H    | 4        | 0.14          |
| (1,1015) | 1:104:A:GLY:H   | 1:110:A:ASP:H    | 5        | 0.14          |
| (1,987)  | 1:117:A:ASP:H   | 1:119:A:MET:H    | 5        | 0.14          |
| (1,966)  | 1:96:A:ALA:H    | 1:94:A:TRP:HZ3   | 2        | 0.14          |
| (1,927)  | 1:49:A:MET:HB3  | 1:49:A:MET:H     | 10       | 0.14          |
| (1,922)  | 1:86:A:ILE:HD13 | 1:88:A:ARG:H     | 2        | 0.14          |
| (1,916)  | 1:122:A:THR:H   | 1:122:A:THR:HG22 | 9        | 0.14          |
| (1,906)  | 1:107:A:GLY:H   | 1:105:A:ARG:H    | 1        | 0.14          |
| (1,904)  | 1:106:A:HIS:HB3 | 1:107:A:GLY:H    | 8        | 0.14          |
| (1,896)  | 1:53:A:ASP:HB3  | 1:53:A:ASP:H     | 9        | 0.14          |
| (1,852)  | 1:114:A:TYR:HB3 | 1:118:A:GLY:H    | 3        | 0.14          |
| (1,852)  | 1:114:A:TYR:HB3 | 1:118:A:GLY:H    | 4        | 0.14          |
| (1,847)  | 1:70:A:LYS:H    | 1:70:A:LYS:HE3   | 1        | 0.14          |
| (1,847)  | 1:70:A:LYS:H    | 1:70:A:LYS:HE3   | 9        | 0.14          |
| (1,822)  | 1:76:A:GLU:HB3  | 1:76:A:GLU:H     | 2        | 0.14          |
| (1,822)  | 1:76:A:GLU:HB3  | 1:76:A:GLU:H     | 7        | 0.14          |
| (1,822)  | 1:76:A:GLU:HB3  | 1:76:A:GLU:H     | 9        | 0.14          |
| (1,776)  | 1:73:A:THR:HB   | 1:61:A:GLU:HG2   | 1        | 0.14          |
| (1,776)  | 1:73:A:THR:HB   | 1:61:A:GLU:HG2   | 5        | 0.14          |
| (1,744)  | 1:86:A:ILE:HG13 | 1:67:A:LEU:HB3   | 3        | 0.14          |
| (1,738)  | 1:78:A:ARG:HD3  | 1:54:A:ASN:H     | 9        | 0.14          |
| (1,721)  | 1:30:A:LYS:HA   | 1:32:A:ASP:H     | 10       | 0.14          |
| (1,689)  | 1:111:A:VAL:HB  | 1:111:A:VAL:H    | 1        | 0.14          |
| (1,649)  | 1:42:A:ALA:HB3  | 1:43:A:LEU:H     | 10       | 0.14          |
| (1,632)  | 1:79:A:SER:HB3  | 1:78:A:ARG:HG3   | 3        | 0.14          |
| (1,614)  | 1:60:A:THR:HA   | 1:100:A:LEU:HD21 | 8        | 0.14          |
| (1,610)  | 1:66:A:ALA:HB2  | 1:62:A:GLN:HE21  | 3        | 0.14          |
| (1,592)  | 1:88:A:ARG:HD3  | 1:88:A:ARG:HA    | 4        | 0.14          |
| (1,592)  | 1:88:A:ARG:HD3  | 1:88:A:ARG:HA    | 10       | 0.14          |
| (1,584)  | 1:100:A:LEU:HA  | 1:112:A:PHE:H    | 8        | 0.14          |
| (1,552)  | 1:85:A:TYR:HB3  | 1:67:A:LEU:HA    | 8        | 0.14          |
| (1,534)  | 1:109:A:VAL:HB  | 1:57:A:TYR:HD2   | 7        | 0.14          |
| (1,525)  | 1:61:A:GLU:HG2  | 1:73:A:THR:HG22  | 7        | 0.14          |
| (1,503)  | 1:88:A:ARG:HB2  | 1:88:A:ARG:HA    | 8        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,474)  | 1:69:A:LYS:HB2  | 1:68:A:VAL:HB    | 2        | 0.14          |
| (1,466)  | 1:82:A:GLN:HG3  | 1:83:A:ASP:H     | 7        | 0.14          |
| (1,367)  | 1:103:A:PRO:HB3 | 1:104:A:GLY:H    | 4        | 0.14          |
| (1,357)  | 1:64:A:LEU:HB2  | 1:64:A:LEU:HD21  | 2        | 0.14          |
| (1,355)  | 1:131:A:VAL:HB  | 1:131:A:VAL:H    | 10       | 0.14          |
| (1,291)  | 1:58:A:PRO:HA   | 1:62:A:GLN:HB2   | 9        | 0.14          |
| (1,270)  | 1:85:A:TYR:HA   | 1:81:A:PRO:HB2   | 6        | 0.14          |
| (1,270)  | 1:85:A:TYR:HA   | 1:81:A:PRO:HB2   | 9        | 0.14          |
| (1,242)  | 1:54:A:ASN:HB2  | 1:77:A:PRO:HA    | 4        | 0.14          |
| (1,242)  | 1:54:A:ASN:HB2  | 1:77:A:PRO:HA    | 8        | 0.14          |
| (1,228)  | 1:63:A:GLY:HA2  | 1:100:A:LEU:HB2  | 10       | 0.14          |
| (1,226)  | 1:60:A:THR:HA   | 1:63:A:GLY:H     | 4        | 0.14          |
| (1,224)  | 1:60:A:THR:HA   | 1:60:A:THR:HG22  | 7        | 0.14          |
| (1,207)  | 1:122:A:THR:HB  | 1:123:A:ASP:HB3  | 3        | 0.14          |
| (1,207)  | 1:122:A:THR:HB  | 1:123:A:ASP:HB3  | 7        | 0.14          |
| (1,207)  | 1:122:A:THR:HB  | 1:123:A:ASP:HB2  | 8        | 0.14          |
| (1,165)  | 1:30:A:LYS:HA   | 1:30:A:LYS:HB2   | 1        | 0.14          |
| (1,165)  | 1:30:A:LYS:HA   | 1:30:A:LYS:HB2   | 5        | 0.14          |
| (1,165)  | 1:30:A:LYS:HA   | 1:30:A:LYS:HB2   | 9        | 0.14          |
| (1,163)  | 1:88:A:ARG:HB3  | 1:88:A:ARG:H     | 1        | 0.14          |
| (1,136)  | 1:50:A:TYR:HA   | 1:54:A:ASN:HB2   | 1        | 0.14          |
| (1,85)   | 1:37:A:ILE:HA   | 1:40:A:ILE:HD13  | 10       | 0.14          |
| (1,75)   | 1:35:A:LYS:HG3  | 1:35:A:LYS:HD2   | 2        | 0.14          |
| (1,75)   | 1:35:A:LYS:HG2  | 1:35:A:LYS:HD3   | 9        | 0.14          |
| (1,54)   | 1:28:A:LYS:HD3  | 1:28:A:LYS:HG2   | 3        | 0.14          |
| (1,54)   | 1:28:A:LYS:HD2  | 1:28:A:LYS:HG3   | 4        | 0.14          |
| (1,30)   | 1:78:A:ARG:HA   | 1:78:A:ARG:HB2   | 6        | 0.14          |
| (1,27)   | 1:31:A:ALA:HA   | 1:31:A:ALA:HB1   | 3        | 0.14          |
| (1,21)   | 1:31:A:ALA:HA   | 1:30:A:LYS:HB3   | 4        | 0.14          |
| (1,11)   | 1:69:A:LYS:HE3  | 1:69:A:LYS:HG2   | 1        | 0.14          |
| (1,10)   | 1:28:A:LYS:HE2  | 1:28:A:LYS:HD2   | 3        | 0.14          |
| (1,10)   | 1:28:A:LYS:HE3  | 1:28:A:LYS:HD2   | 4        | 0.14          |
| (1,6)    | 1:130:A:ASN:HB2 | 1:131:A:VAL:HG12 | 4        | 0.14          |
| (1,1594) | 1:54:A:ASN:H    | 1:51:A:LYS:HB2   | 5        | 0.13          |
| (1,1563) | 1:100:A:LEU:HG  | 1:102:A:SER:H    | 5        | 0.13          |
| (1,1540) | 1:57:A:TYR:H    | 1:56:A:ARG:H     | 1        | 0.13          |
| (1,1508) | 1:66:A:ALA:HA   | 1:69:A:LYS:H     | 7        | 0.13          |
| (1,1507) | 1:58:A:PRO:HB2  | 1:100:A:LEU:HD22 | 7        | 0.13          |
| (1,1502) | 1:57:A:TYR:HA   | 1:57:A:TYR:HD2   | 4        | 0.13          |
| (1,1484) | 1:64:A:LEU:HD22 | 1:63:A:GLY:HA2   | 2        | 0.13          |
| (1,1462) | 1:45:A:SER:HB2  | 1:44:A:GLU:HB3   | 3        | 0.13          |
| (1,1398) | 1:51:A:LYS:H    | 1:57:A:TYR:HD2   | 6        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1385) | 1:36:A:ALA:H     | 1:35:A:LYS:HG3   | 2        | 0.13          |
| (1,1352) | 1:52:A:LEU:H     | 1:50:A:TYR:HD2   | 5        | 0.13          |
| (1,1249) | 1:94:A:TRP:HE1   | 1:116:A:PRO:HB2  | 4        | 0.13          |
| (1,1232) | 1:50:A:TYR:H     | 1:85:A:TYR:HE2   | 8        | 0.13          |
| (1,1224) | 1:122:A:THR:H    | 1:120:A:PRO:HB2  | 3        | 0.13          |
| (1,1218) | 1:115:A:GLY:H    | 1:114:A:TYR:HB3  | 1        | 0.13          |
| (1,1218) | 1:115:A:GLY:H    | 1:114:A:TYR:HB3  | 8        | 0.13          |
| (1,1218) | 1:115:A:GLY:H    | 1:114:A:TYR:HB3  | 10       | 0.13          |
| (1,1091) | 1:32:A:ASP:H     | 1:28:A:LYS:HG3   | 1        | 0.13          |
| (1,1091) | 1:32:A:ASP:H     | 1:28:A:LYS:HG3   | 6        | 0.13          |
| (1,1087) | 1:113:A:SER:H    | 1:112:A:PHE:HB3  | 6        | 0.13          |
| (1,1049) | 1:51:A:LYS:HG2   | 1:56:A:ARG:H     | 10       | 0.13          |
| (1,1043) | 1:100:A:LEU:H    | 1:111:A:VAL:HG13 | 5        | 0.13          |
| (1,1041) | 1:100:A:LEU:HB2  | 1:100:A:LEU:H    | 1        | 0.13          |
| (1,1015) | 1:104:A:GLY:H    | 1:110:A:ASP:H    | 6        | 0.13          |
| (1,1015) | 1:104:A:GLY:H    | 1:110:A:ASP:H    | 10       | 0.13          |
| (1,985)  | 1:119:A:MET:H    | 1:122:A:THR:HG21 | 7        | 0.13          |
| (1,922)  | 1:86:A:ILE:HD12  | 1:88:A:ARG:H     | 8        | 0.13          |
| (1,916)  | 1:122:A:THR:H    | 1:122:A:THR:HG22 | 1        | 0.13          |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG21  | 6        | 0.13          |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG22  | 8        | 0.13          |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG22  | 9        | 0.13          |
| (1,852)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:H    | 5        | 0.13          |
| (1,852)  | 1:114:A:TYR:HB3  | 1:118:A:GLY:H    | 10       | 0.13          |
| (1,822)  | 1:76:A:GLU:HB3   | 1:76:A:GLU:H     | 5        | 0.13          |
| (1,799)  | 1:94:A:TRP:HZ2   | 1:32:A:ASP:HB3   | 7        | 0.13          |
| (1,783)  | 1:125:A:ASP:HA   | 1:126:A:ILE:HB   | 6        | 0.13          |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2   | 4        | 0.13          |
| (1,776)  | 1:73:A:THR:HB    | 1:61:A:GLU:HG2   | 7        | 0.13          |
| (1,750)  | 1:53:A:ASP:HB2   | 1:85:A:TYR:HD1   | 2        | 0.13          |
| (1,750)  | 1:53:A:ASP:HB2   | 1:85:A:TYR:HD1   | 3        | 0.13          |
| (1,689)  | 1:111:A:VAL:HB   | 1:111:A:VAL:H    | 4        | 0.13          |
| (1,663)  | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2   | 6        | 0.13          |
| (1,657)  | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD13  | 5        | 0.13          |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H     | 1        | 0.13          |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H     | 2        | 0.13          |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H     | 3        | 0.13          |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H     | 5        | 0.13          |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H     | 6        | 0.13          |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H     | 9        | 0.13          |
| (1,629)  | 1:65:A:GLY:HA2   | 1:65:A:GLY:H     | 10       | 0.13          |
| (1,592)  | 1:88:A:ARG:HD3   | 1:88:A:ARG:HA    | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 3        | 0.13          |
| (1,584)  | 1:100:A:LEU:HA   | 1:112:A:PHE:H    | 9        | 0.13          |
| (1,552)  | 1:85:A:TYR:HB3   | 1:67:A:LEU:HA    | 1        | 0.13          |
| (1,514)  | 1:51:A:LYS:HG3   | 1:56:A:ARG:HA    | 2        | 0.13          |
| (1,502)  | 1:46:A:ALA:HA    | 1:85:A:TYR:HB2   | 9        | 0.13          |
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG22  | 6        | 0.13          |
| (1,483)  | 1:59:A:THR:HG23  | 1:58:A:PRO:HA    | 2        | 0.13          |
| (1,466)  | 1:82:A:GLN:HG2   | 1:83:A:ASP:H     | 4        | 0.13          |
| (1,466)  | 1:82:A:GLN:HG2   | 1:83:A:ASP:H     | 10       | 0.13          |
| (1,451)  | 1:109:A:VAL:HG12 | 1:100:A:LEU:HD11 | 4        | 0.13          |
| (1,435)  | 1:41:A:VAL:HG13  | 1:42:A:ALA:H     | 5        | 0.13          |
| (1,420)  | 1:48:A:ASP:HA    | 1:57:A:TYR:HE2   | 10       | 0.13          |
| (1,367)  | 1:103:A:PRO:HB3  | 1:104:A:GLY:H    | 5        | 0.13          |
| (1,350)  | 1:112:A:PHE:HA   | 1:112:A:PHE:HD1  | 1        | 0.13          |
| (1,350)  | 1:112:A:PHE:HA   | 1:112:A:PHE:HD1  | 2        | 0.13          |
| (1,350)  | 1:112:A:PHE:HA   | 1:112:A:PHE:HD2  | 6        | 0.13          |
| (1,350)  | 1:112:A:PHE:HA   | 1:112:A:PHE:HD1  | 7        | 0.13          |
| (1,332)  | 1:112:A:PHE:HB2  | 1:129:A:TRP:HZ3  | 4        | 0.13          |
| (1,332)  | 1:112:A:PHE:HB2  | 1:129:A:TRP:HZ3  | 6        | 0.13          |
| (1,298)  | 1:101:A:VAL:HG13 | 1:110:A:ASP:HB2  | 5        | 0.13          |
| (1,298)  | 1:101:A:VAL:HG13 | 1:110:A:ASP:HB2  | 10       | 0.13          |
| (1,282)  | 1:78:A:ARG:HD3   | 1:78:A:ARG:HG3   | 5        | 0.13          |
| (1,228)  | 1:63:A:GLY:HA2   | 1:100:A:LEU:HB2  | 5        | 0.13          |
| (1,226)  | 1:60:A:THR:HA    | 1:63:A:GLY:H     | 1        | 0.13          |
| (1,226)  | 1:60:A:THR:HA    | 1:63:A:GLY:H     | 6        | 0.13          |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG22  | 3        | 0.13          |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG21  | 4        | 0.13          |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG21  | 10       | 0.13          |
| (1,195)  | 1:111:A:VAL:HG11 | 1:44:A:GLU:HA    | 8        | 0.13          |
| (1,185)  | 1:91:A:GLN:HA    | 1:91:A:GLN:HG3   | 2        | 0.13          |
| (1,165)  | 1:30:A:LYS:HA    | 1:30:A:LYS:HB2   | 4        | 0.13          |
| (1,106)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HD11  | 1        | 0.13          |
| (1,75)   | 1:35:A:LYS:HG3   | 1:35:A:LYS:HD2   | 6        | 0.13          |
| (1,54)   | 1:28:A:LYS:HD2   | 1:28:A:LYS:HG3   | 2        | 0.13          |
| (1,54)   | 1:28:A:LYS:HD2   | 1:28:A:LYS:HG3   | 10       | 0.13          |
| (1,30)   | 1:78:A:ARG:HA    | 1:78:A:ARG:HB3   | 10       | 0.13          |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB1   | 2        | 0.13          |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG13 | 1        | 0.13          |
| (1,6)    | 1:130:A:ASN:HB2  | 1:131:A:VAL:HG13 | 6        | 0.13          |
| (1,1576) | 1:83:A:ASP:H     | 1:84:A:GLY:HA3   | 3        | 0.12          |
| (1,1570) | 1:79:A:SER:H     | 1:53:A:ASP:HB3   | 10       | 0.12          |
| (1,1563) | 1:100:A:LEU:HG   | 1:102:A:SER:H    | 3        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1563) | 1:100:A:LEU:HG  | 1:102:A:SER:H    | 8        | 0.12          |
| (1,1561) | 1:52:A:LEU:H    | 1:51:A:LYS:HB3   | 7        | 0.12          |
| (1,1508) | 1:66:A:ALA:HA   | 1:69:A:LYS:H     | 5        | 0.12          |
| (1,1454) | 1:40:A:ILE:HB   | 1:111:A:VAL:HG23 | 9        | 0.12          |
| (1,1452) | 1:37:A:ILE:HA   | 1:37:A:ILE:HD13  | 5        | 0.12          |
| (1,1283) | 1:73:A:THR:H    | 1:62:A:GLN:HB3   | 1        | 0.12          |
| (1,1087) | 1:113:A:SER:H   | 1:112:A:PHE:HB3  | 2        | 0.12          |
| (1,1087) | 1:113:A:SER:H   | 1:112:A:PHE:HB3  | 5        | 0.12          |
| (1,1087) | 1:113:A:SER:H   | 1:112:A:PHE:HB3  | 8        | 0.12          |
| (1,1015) | 1:104:A:GLY:H   | 1:110:A:ASP:H    | 8        | 0.12          |
| (1,1006) | 1:108:A:LYS:HB2 | 1:109:A:VAL:H    | 5        | 0.12          |
| (1,922)  | 1:86:A:ILE:HD11 | 1:88:A:ARG:H     | 9        | 0.12          |
| (1,915)  | 1:122:A:THR:H   | 1:121:A:ASP:HB3  | 5        | 0.12          |
| (1,915)  | 1:122:A:THR:H   | 1:121:A:ASP:HB3  | 7        | 0.12          |
| (1,906)  | 1:107:A:GLY:H   | 1:105:A:ARG:H    | 8        | 0.12          |
| (1,904)  | 1:106:A:HIS:HB3 | 1:107:A:GLY:H    | 5        | 0.12          |
| (1,902)  | 1:107:A:GLY:H   | 1:104:A:GLY:HA3  | 4        | 0.12          |
| (1,896)  | 1:53:A:ASP:HB3  | 1:53:A:ASP:H     | 4        | 0.12          |
| (1,879)  | 1:48:A:ASP:H    | 1:44:A:GLU:HA    | 7        | 0.12          |
| (1,875)  | 1:61:A:GLU:H    | 1:60:A:THR:HG22  | 4        | 0.12          |
| (1,875)  | 1:61:A:GLU:H    | 1:60:A:THR:HG23  | 7        | 0.12          |
| (1,875)  | 1:61:A:GLU:H    | 1:60:A:THR:HG22  | 10       | 0.12          |
| (1,822)  | 1:76:A:GLU:HB3  | 1:76:A:GLU:H     | 3        | 0.12          |
| (1,822)  | 1:76:A:GLU:HB3  | 1:76:A:GLU:H     | 10       | 0.12          |
| (1,804)  | 1:122:A:THR:HA  | 1:121:A:ASP:HA   | 1        | 0.12          |
| (1,783)  | 1:125:A:ASP:HA  | 1:126:A:ILE:HB   | 1        | 0.12          |
| (1,780)  | 1:85:A:TYR:HB3  | 1:67:A:LEU:HD11  | 2        | 0.12          |
| (1,750)  | 1:53:A:ASP:HB2  | 1:85:A:TYR:HD2   | 5        | 0.12          |
| (1,726)  | 1:101:A:VAL:HB  | 1:100:A:LEU:HA   | 9        | 0.12          |
| (1,721)  | 1:30:A:LYS:HA   | 1:32:A:ASP:H     | 7        | 0.12          |
| (1,689)  | 1:111:A:VAL:HB  | 1:111:A:VAL:H    | 5        | 0.12          |
| (1,689)  | 1:111:A:VAL:HB  | 1:111:A:VAL:H    | 10       | 0.12          |
| (1,649)  | 1:42:A:ALA:HB1  | 1:43:A:LEU:H     | 1        | 0.12          |
| (1,649)  | 1:42:A:ALA:HB3  | 1:43:A:LEU:H     | 4        | 0.12          |
| (1,629)  | 1:65:A:GLY:HA2  | 1:65:A:GLY:H     | 4        | 0.12          |
| (1,629)  | 1:65:A:GLY:HA2  | 1:65:A:GLY:H     | 7        | 0.12          |
| (1,629)  | 1:65:A:GLY:HA2  | 1:65:A:GLY:H     | 8        | 0.12          |
| (1,595)  | 1:123:A:ASP:HA  | 1:123:A:ASP:HB2  | 9        | 0.12          |
| (1,552)  | 1:85:A:TYR:HB3  | 1:67:A:LEU:HA    | 9        | 0.12          |
| (1,548)  | 1:43:A:LEU:HA   | 1:46:A:ALA:HB2   | 10       | 0.12          |
| (1,534)  | 1:109:A:VAL:HB  | 1:57:A:TYR:HD1   | 1        | 0.12          |
| (1,534)  | 1:109:A:VAL:HB  | 1:57:A:TYR:HD2   | 3        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,486)  | 1:75:A:PRO:HG2   | 1:59:A:THR:HG23  | 5        | 0.12          |
| (1,464)  | 1:82:A:GLN:HG3   | 1:82:A:GLN:HA    | 7        | 0.12          |
| (1,367)  | 1:103:A:PRO:HB3  | 1:104:A:GLY:H    | 10       | 0.12          |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD21  | 5        | 0.12          |
| (1,350)  | 1:112:A:PHE:HA   | 1:112:A:PHE:HD2  | 5        | 0.12          |
| (1,324)  | 1:53:A:ASP:HB3   | 1:79:A:SER:HB2   | 4        | 0.12          |
| (1,298)  | 1:101:A:VAL:HG13 | 1:110:A:ASP:HB2  | 3        | 0.12          |
| (1,298)  | 1:101:A:VAL:HG12 | 1:110:A:ASP:HB2  | 4        | 0.12          |
| (1,275)  | 1:119:A:MET:HB3  | 1:122:A:THR:HG23 | 10       | 0.12          |
| (1,226)  | 1:60:A:THR:HA    | 1:63:A:GLY:H     | 8        | 0.12          |
| (1,226)  | 1:60:A:THR:HA    | 1:63:A:GLY:H     | 9        | 0.12          |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG23  | 1        | 0.12          |
| (1,224)  | 1:60:A:THR:HA    | 1:60:A:THR:HG21  | 2        | 0.12          |
| (1,156)  | 1:80:A:TYR:HB2   | 1:85:A:TYR:HD2   | 9        | 0.12          |
| (1,133)  | 1:41:A:VAL:HG23  | 1:41:A:VAL:H     | 6        | 0.12          |
| (1,128)  | 1:41:A:VAL:HA    | 1:44:A:GLU:HB3   | 1        | 0.12          |
| (1,106)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HD12  | 4        | 0.12          |
| (1,75)   | 1:35:A:LYS:HG3   | 1:35:A:LYS:HD2   | 1        | 0.12          |
| (1,54)   | 1:28:A:LYS:HD3   | 1:28:A:LYS:HG2   | 8        | 0.12          |
| (1,41)   | 1:108:A:LYS:HA   | 1:109:A:VAL:H    | 2        | 0.12          |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB1   | 6        | 0.12          |
| (1,10)   | 1:28:A:LYS:HE3   | 1:28:A:LYS:HD3   | 1        | 0.12          |
| (1,10)   | 1:28:A:LYS:HE3   | 1:28:A:LYS:HD3   | 10       | 0.12          |
| (1,1575) | 1:118:A:GLY:H    | 1:114:A:TYR:HD1  | 5        | 0.11          |
| (1,1570) | 1:79:A:SER:H     | 1:53:A:ASP:HB3   | 6        | 0.11          |
| (1,1507) | 1:58:A:PRO:HB2   | 1:100:A:LEU:HD21 | 1        | 0.11          |
| (1,1497) | 1:73:A:THR:HB    | 1:62:A:GLN:HG2   | 4        | 0.11          |
| (1,1497) | 1:73:A:THR:HB    | 1:62:A:GLN:HG2   | 6        | 0.11          |
| (1,1466) | 1:64:A:LEU:HB2   | 1:99:A:GLN:HA    | 9        | 0.11          |
| (1,1454) | 1:40:A:ILE:HB    | 1:111:A:VAL:HG23 | 5        | 0.11          |
| (1,1452) | 1:37:A:ILE:HA    | 1:37:A:ILE:HD13  | 10       | 0.11          |
| (1,1441) | 1:79:A:SER:H     | 1:85:A:TYR:HE2   | 4        | 0.11          |
| (1,1398) | 1:51:A:LYS:H     | 1:57:A:TYR:HD2   | 4        | 0.11          |
| (1,1380) | 1:132:A:GLY:HA2  | 1:40:A:ILE:H     | 7        | 0.11          |
| (1,1348) | 1:126:A:ILE:H    | 1:112:A:PHE:HD1  | 6        | 0.11          |
| (1,1283) | 1:73:A:THR:H     | 1:62:A:GLN:HB3   | 8        | 0.11          |
| (1,1164) | 1:79:A:SER:H     | 1:78:A:ARG:HG3   | 2        | 0.11          |
| (1,1091) | 1:32:A:ASP:H     | 1:28:A:LYS:HG3   | 2        | 0.11          |
| (1,1087) | 1:113:A:SER:H    | 1:112:A:PHE:HB3  | 9        | 0.11          |
| (1,1053) | 1:53:A:ASP:HB3   | 1:54:A:ASN:H     | 1        | 0.11          |
| (1,987)  | 1:117:A:ASP:H    | 1:119:A:MET:H    | 1        | 0.11          |
| (1,987)  | 1:117:A:ASP:H    | 1:119:A:MET:H    | 7        | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,984) | 1:96:A:ALA:HB1   | 1:97:A:GLU:H    | 2        | 0.11          |
| (1,922) | 1:86:A:ILE:HD11  | 1:88:A:ARG:H    | 1        | 0.11          |
| (1,915) | 1:122:A:THR:H    | 1:121:A:ASP:HB3 | 8        | 0.11          |
| (1,896) | 1:53:A:ASP:HB3   | 1:53:A:ASP:H    | 5        | 0.11          |
| (1,880) | 1:29:A:GLU:H     | 1:29:A:GLU:HG3  | 1        | 0.11          |
| (1,879) | 1:48:A:ASP:H     | 1:44:A:GLU:HA   | 2        | 0.11          |
| (1,879) | 1:48:A:ASP:H     | 1:44:A:GLU:HA   | 4        | 0.11          |
| (1,832) | 1:119:A:MET:H    | 1:119:A:MET:HG3 | 8        | 0.11          |
| (1,822) | 1:76:A:GLU:HB3   | 1:76:A:GLU:H    | 1        | 0.11          |
| (1,817) | 1:56:A:ARG:H     | 1:56:A:ARG:HD3  | 7        | 0.11          |
| (1,784) | 1:114:A:TYR:HA   | 1:126:A:ILE:HB  | 6        | 0.11          |
| (1,766) | 1:131:A:VAL:HG21 | 1:128:A:ASN:HB3 | 10       | 0.11          |
| (1,750) | 1:53:A:ASP:HB2   | 1:85:A:TYR:HD1  | 10       | 0.11          |
| (1,721) | 1:30:A:LYS:HA    | 1:32:A:ASP:H    | 4        | 0.11          |
| (1,721) | 1:30:A:LYS:HA    | 1:32:A:ASP:H    | 6        | 0.11          |
| (1,704) | 1:104:A:GLY:HA3  | 1:106:A:HIS:H   | 8        | 0.11          |
| (1,704) | 1:104:A:GLY:HA3  | 1:106:A:HIS:H   | 10       | 0.11          |
| (1,689) | 1:111:A:VAL:HB   | 1:111:A:VAL:H   | 2        | 0.11          |
| (1,689) | 1:111:A:VAL:HB   | 1:111:A:VAL:H   | 6        | 0.11          |
| (1,689) | 1:111:A:VAL:HB   | 1:111:A:VAL:H   | 7        | 0.11          |
| (1,689) | 1:111:A:VAL:HB   | 1:111:A:VAL:H   | 8        | 0.11          |
| (1,663) | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2  | 3        | 0.11          |
| (1,663) | 1:85:A:TYR:HA    | 1:85:A:TYR:HD2  | 4        | 0.11          |
| (1,657) | 1:111:A:VAL:HG22 | 1:43:A:LEU:HD13 | 2        | 0.11          |
| (1,655) | 1:56:A:ARG:HB3   | 1:57:A:TYR:H    | 3        | 0.11          |
| (1,655) | 1:56:A:ARG:HB3   | 1:57:A:TYR:H    | 7        | 0.11          |
| (1,649) | 1:42:A:ALA:HB3   | 1:43:A:LEU:H    | 5        | 0.11          |
| (1,649) | 1:42:A:ALA:HB2   | 1:43:A:LEU:H    | 7        | 0.11          |
| (1,649) | 1:42:A:ALA:HB3   | 1:43:A:LEU:H    | 9        | 0.11          |
| (1,634) | 1:79:A:SER:HB3   | 1:54:A:ASN:HA   | 9        | 0.11          |
| (1,466) | 1:82:A:GLN:HG2   | 1:83:A:ASP:H    | 5        | 0.11          |
| (1,464) | 1:82:A:GLN:HG3   | 1:82:A:GLN:HA   | 3        | 0.11          |
| (1,434) | 1:41:A:VAL:HG11  | 1:38:A:SER:H    | 3        | 0.11          |
| (1,350) | 1:112:A:PHE:HA   | 1:112:A:PHE:HD1 | 10       | 0.11          |
| (1,325) | 1:79:A:SER:HB2   | 1:79:A:SER:H    | 9        | 0.11          |
| (1,322) | 1:52:A:LEU:HG    | 1:136:A:HIS:HD2 | 8        | 0.11          |
| (1,313) | 1:69:A:LYS:HG2   | 1:69:A:LYS:HA   | 5        | 0.11          |
| (1,291) | 1:58:A:PRO:HA    | 1:62:A:GLN:HB2  | 3        | 0.11          |
| (1,246) | 1:120:A:PRO:HA   | 1:122:A:THR:H   | 10       | 0.11          |
| (1,224) | 1:60:A:THR:HA    | 1:60:A:THR:HG21 | 9        | 0.11          |
| (1,186) | 1:46:A:ALA:HA    | 1:46:A:ALA:HB1  | 4        | 0.11          |
| (1,186) | 1:46:A:ALA:HA    | 1:46:A:ALA:HB3  | 6        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,156)  | 1:80:A:TYR:HB2   | 1:85:A:TYR:HD2   | 8        | 0.11          |
| (1,128)  | 1:41:A:VAL:HA    | 1:44:A:GLU:HB3   | 9        | 0.11          |
| (1,106)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HD13  | 5        | 0.11          |
| (1,106)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HD13  | 6        | 0.11          |
| (1,106)  | 1:40:A:ILE:HA    | 1:40:A:ILE:HD11  | 8        | 0.11          |
| (1,30)   | 1:78:A:ARG:HA    | 1:78:A:ARG:HB3   | 8        | 0.11          |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB3   | 1        | 0.11          |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB2   | 5        | 0.11          |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB1   | 7        | 0.11          |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB1   | 8        | 0.11          |
| (1,27)   | 1:31:A:ALA:HA    | 1:31:A:ALA:HB2   | 9        | 0.11          |
| (1,1595) | 1:32:A:ASP:H     | 1:30:A:LYS:HB3   | 1        | 0.1           |
| (1,1540) | 1:57:A:TYR:H     | 1:56:A:ARG:H     | 6        | 0.1           |
| (1,1540) | 1:57:A:TYR:H     | 1:56:A:ARG:H     | 10       | 0.1           |
| (1,1481) | 1:37:A:ILE:HG21  | 1:131:A:VAL:HB   | 10       | 0.1           |
| (1,1477) | 1:133:A:THR:HB   | 1:133:A:THR:HG22 | 4        | 0.1           |
| (1,1459) | 1:86:A:ILE:HB    | 1:86:A:ILE:HG21  | 1        | 0.1           |
| (1,1349) | 1:52:A:LEU:H     | 1:48:A:ASP:HB3   | 10       | 0.1           |
| (1,1348) | 1:126:A:ILE:H    | 1:112:A:PHE:HD2  | 7        | 0.1           |
| (1,1230) | 1:49:A:MET:H     | 1:47:A:LEU:HB2   | 10       | 0.1           |
| (1,1218) | 1:115:A:GLY:H    | 1:114:A:TYR:HB3  | 9        | 0.1           |
| (1,1015) | 1:104:A:GLY:H    | 1:110:A:ASP:H    | 1        | 0.1           |
| (1,1015) | 1:104:A:GLY:H    | 1:110:A:ASP:H    | 9        | 0.1           |
| (1,987)  | 1:117:A:ASP:H    | 1:119:A:MET:H    | 9        | 0.1           |
| (1,922)  | 1:86:A:ILE:HD12  | 1:88:A:ARG:H     | 3        | 0.1           |
| (1,922)  | 1:86:A:ILE:HD12  | 1:88:A:ARG:H     | 6        | 0.1           |
| (1,915)  | 1:122:A:THR:H    | 1:121:A:ASP:HB3  | 4        | 0.1           |
| (1,915)  | 1:122:A:THR:H    | 1:121:A:ASP:HB3  | 6        | 0.1           |
| (1,915)  | 1:122:A:THR:H    | 1:121:A:ASP:HB3  | 9        | 0.1           |
| (1,915)  | 1:122:A:THR:H    | 1:121:A:ASP:HB3  | 10       | 0.1           |
| (1,902)  | 1:107:A:GLY:H    | 1:104:A:GLY:HA3  | 10       | 0.1           |
| (1,875)  | 1:61:A:GLU:H     | 1:60:A:THR:HG23  | 3        | 0.1           |
| (1,817)  | 1:56:A:ARG:H     | 1:56:A:ARG:HD3   | 2        | 0.1           |
| (1,766)  | 1:131:A:VAL:HG23 | 1:128:A:ASN:HB3  | 3        | 0.1           |
| (1,750)  | 1:53:A:ASP:HB2   | 1:85:A:TYR:HD1   | 4        | 0.1           |
| (1,704)  | 1:104:A:GLY:HA3  | 1:106:A:HIS:H    | 3        | 0.1           |
| (1,689)  | 1:111:A:VAL:HB   | 1:111:A:VAL:H    | 3        | 0.1           |
| (1,689)  | 1:111:A:VAL:HB   | 1:111:A:VAL:H    | 9        | 0.1           |
| (1,552)  | 1:85:A:TYR:HB3   | 1:67:A:LEU:HA    | 6        | 0.1           |
| (1,421)  | 1:129:A:TRP:HB2  | 1:106:A:HIS:HB2  | 4        | 0.1           |
| (1,367)  | 1:103:A:PRO:HB3  | 1:104:A:GLY:H    | 1        | 0.1           |
| (1,357)  | 1:64:A:LEU:HB2   | 1:64:A:LEU:HD23  | 3        | 0.1           |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,350) | 1:112:A:PHE:HA  | 1:112:A:PHE:HD1  | 4        | 0.1           |
| (1,332) | 1:112:A:PHE:HB2 | 1:129:A:TRP:HZ3  | 3        | 0.1           |
| (1,226) | 1:60:A:THR:HA   | 1:63:A:GLY:H     | 2        | 0.1           |
| (1,224) | 1:60:A:THR:HA   | 1:60:A:THR:HG21  | 8        | 0.1           |
| (1,149) | 1:54:A:ASN:HB3  | 1:78:A:ARG:H     | 5        | 0.1           |
| (1,136) | 1:50:A:TYR:HA   | 1:54:A:ASN:HB2   | 10       | 0.1           |
| (1,133) | 1:41:A:VAL:HG21 | 1:41:A:VAL:H     | 3        | 0.1           |
| (1,90)  | 1:34:A:GLN:HG2  | 1:37:A:ILE:HD11  | 2        | 0.1           |
| (1,27)  | 1:31:A:ALA:HA   | 1:31:A:ALA:HB2   | 10       | 0.1           |
| (1,11)  | 1:69:A:LYS:HE2  | 1:69:A:LYS:HG2   | 6        | 0.1           |
| (1,6)   | 1:130:A:ASN:HB2 | 1:131:A:VAL:HG13 | 2        | 0.1           |

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

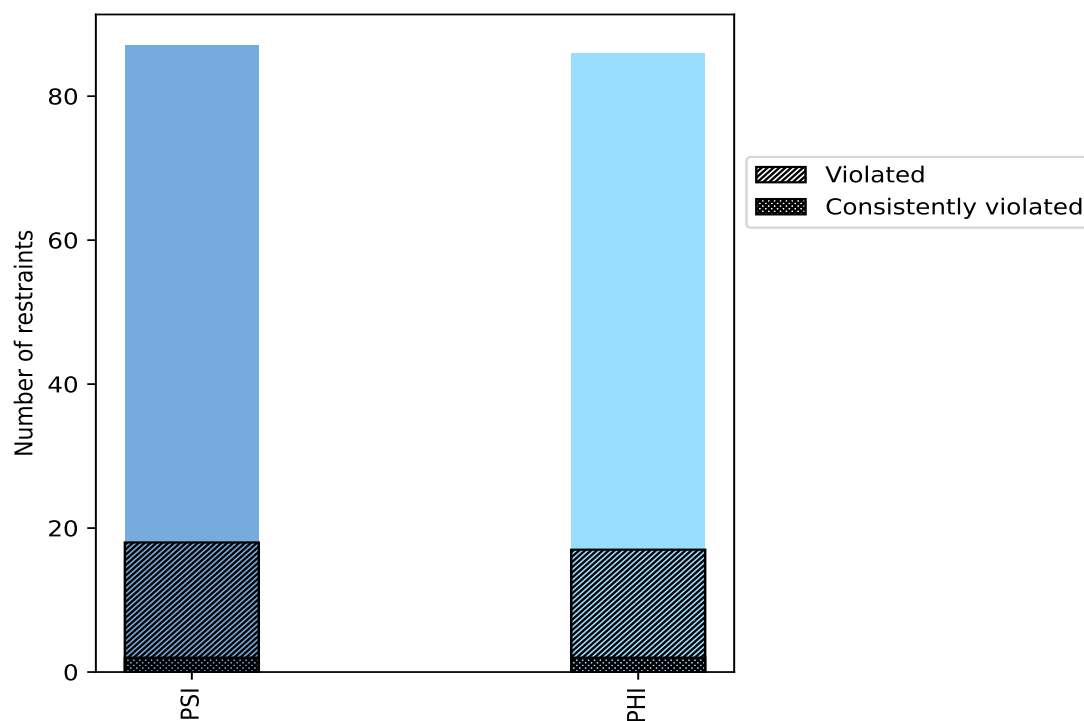
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 87    | 50.3           | 18                    | 20.7           | 10.4           | 2                                  | 2.3            | 1.2            |
| PHI        | 86    | 49.7           | 17                    | 19.8           | 9.8            | 2                                  | 2.3            | 1.2            |
| Total      | 173   | 100.0          | 35                    | 20.2           | 20.2           | 4                                  | 2.3            | 2.3            |

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

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



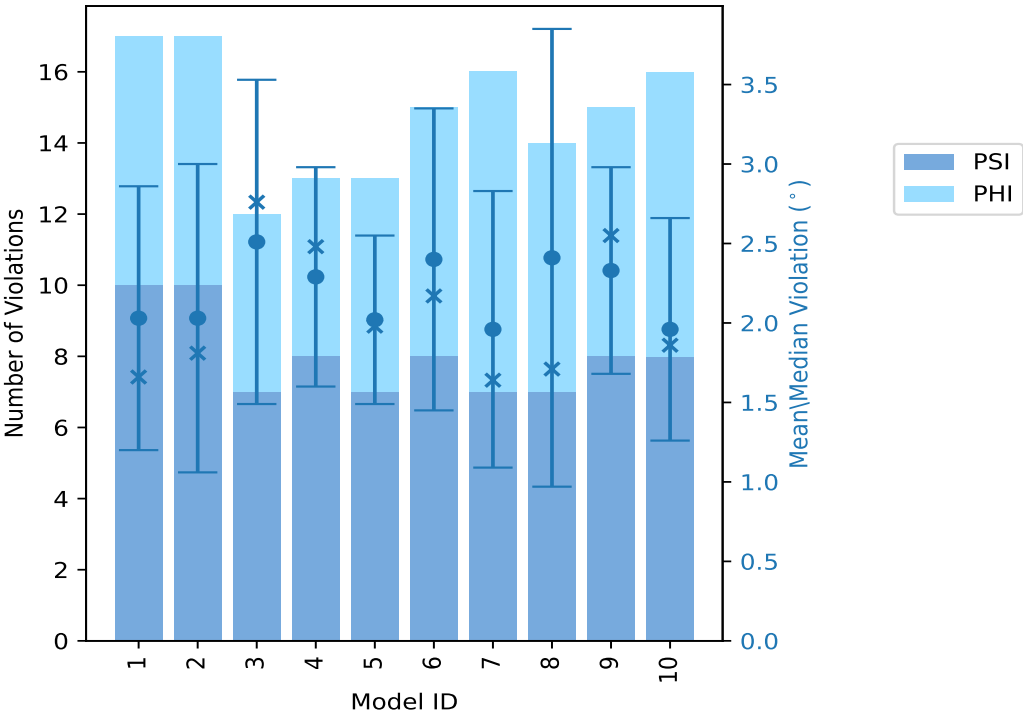
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 10                   | 7   | 17    | 2.03     | 4.08    | 0.83   | 1.66       |
| 2        | 10                   | 7   | 17    | 2.03     | 5.1     | 0.97   | 1.81       |
| 3        | 7                    | 5   | 12    | 2.51     | 4.19    | 1.02   | 2.76       |
| 4        | 8                    | 5   | 13    | 2.29     | 3.33    | 0.69   | 2.48       |
| 5        | 7                    | 6   | 13    | 2.02     | 2.76    | 0.53   | 1.98       |
| 6        | 8                    | 7   | 15    | 2.4      | 4.69    | 0.95   | 2.17       |
| 7        | 7                    | 9   | 16    | 1.96     | 4.05    | 0.87   | 1.64       |
| 8        | 7                    | 7   | 14    | 2.41     | 6.23    | 1.44   | 1.71       |
| 9        | 8                    | 7   | 15    | 2.33     | 3.41    | 0.65   | 2.55       |
| 10       | 8                    | 8   | 16    | 1.96     | 3.6     | 0.7    | 1.86       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

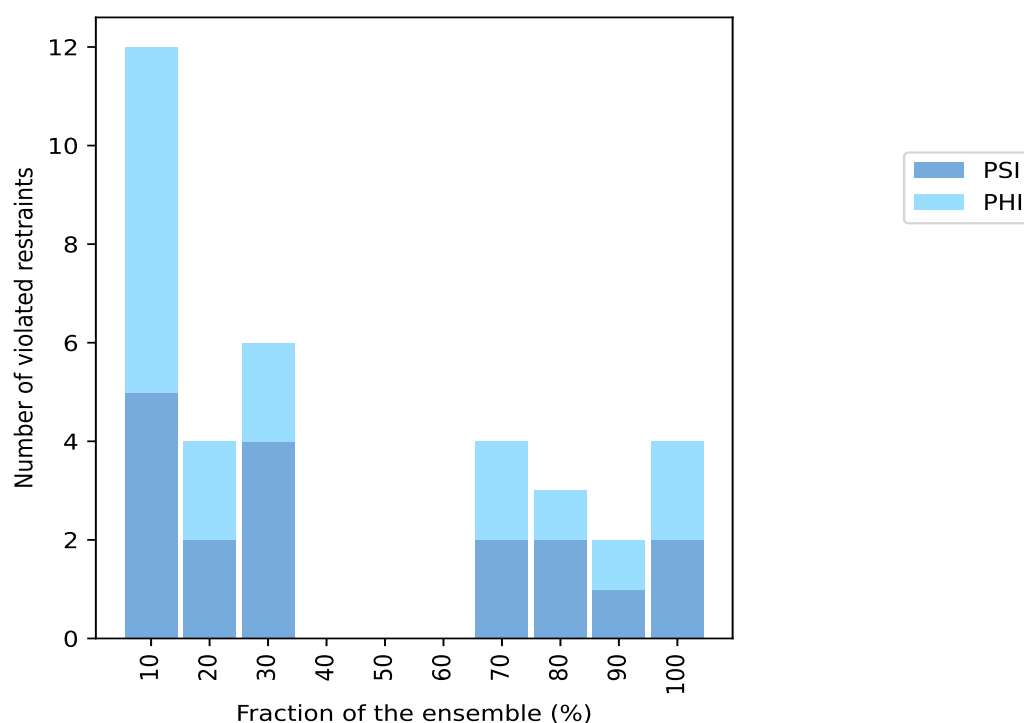
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

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

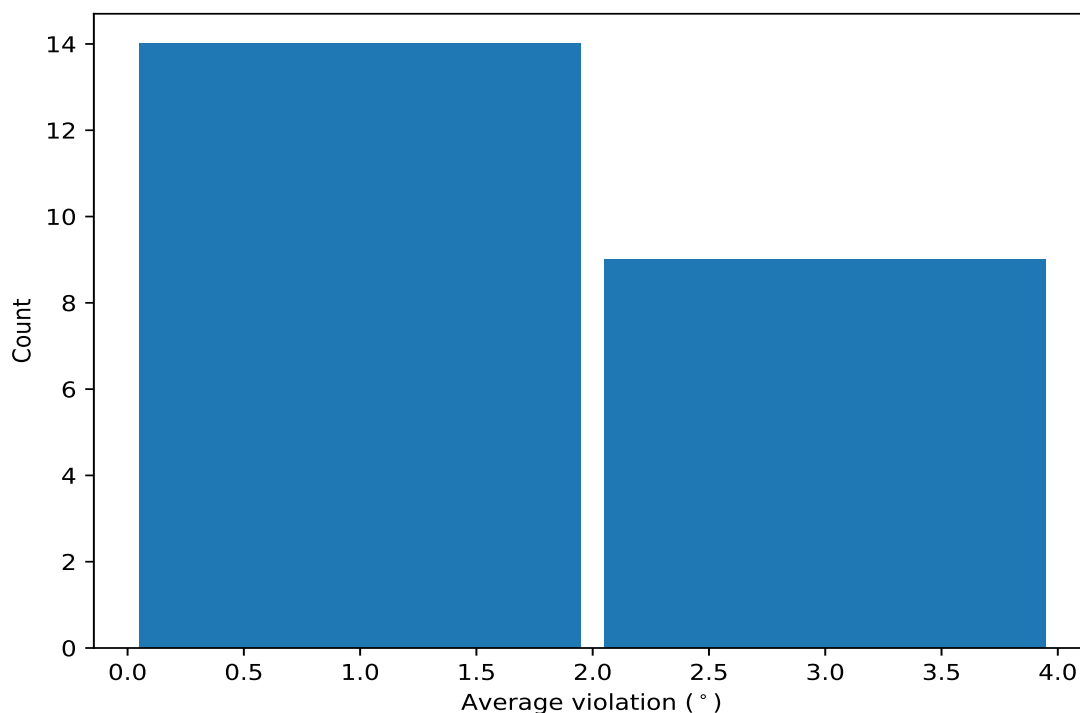
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 10                  | 3.38 | 0.96            | 3.1    |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 10                  | 3.14 | 0.6             | 3.02   |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 10                  | 3.01 | 0.57            | 3.04   |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 10                  | 2.5  | 0.45            | 2.32   |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 9                   | 2.49 | 0.66            | 2.68   |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 9                   | 2.37 | 0.48            | 2.61   |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 8                   | 2.12 | 0.7             | 2.27   |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 8                   | 1.97 | 0.62            | 1.74   |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 8                   | 1.7  | 0.48            | 1.58   |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 7                   | 1.9  | 0.44            | 1.85   |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 7                   | 1.67 | 0.26            | 1.81   |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 7                   | 1.66 | 0.36            | 1.55   |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 7                   | 1.32 | 0.24            | 1.32   |

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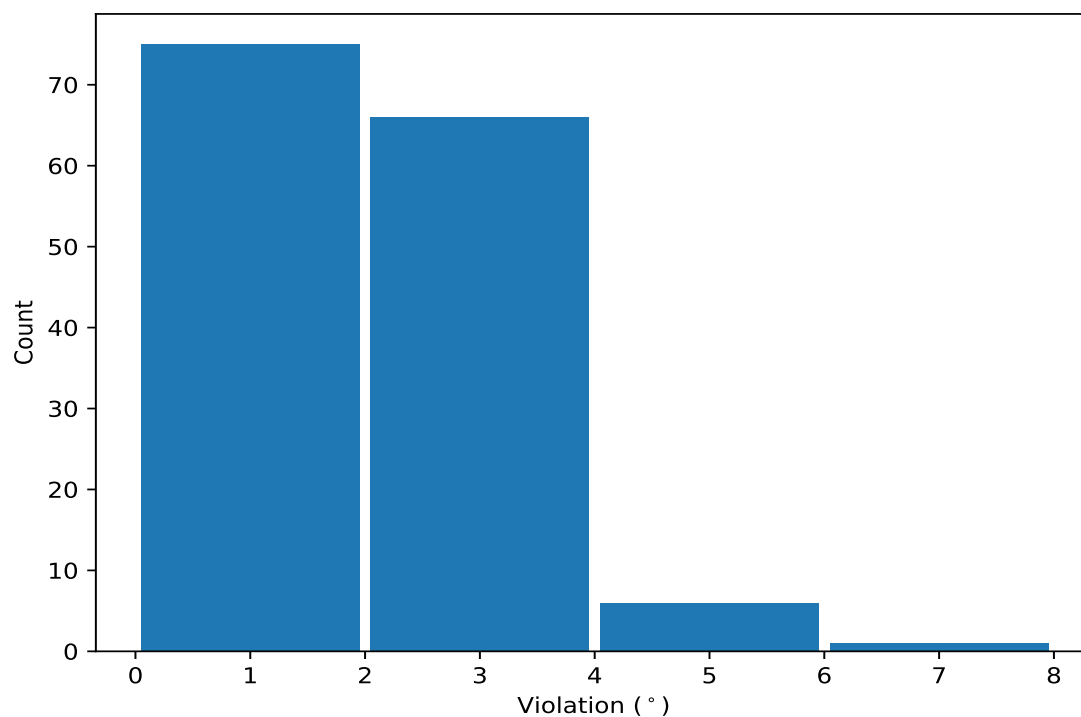
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,156) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C  | 1:125:A:ASP:N | 3                   | 2.59 | 1.5             | 1.78   |
| (1,173) | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C  | 1:118:A:GLY:N | 3                   | 2.16 | 0.62            | 2.2    |
| (1,81)  | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C   | 1:71:A:PRO:N  | 3                   | 1.63 | 0.39            | 1.53   |
| (1,151) | 1:121:A:ASP:C | 1:122:A:THR:N  | 1:122:A:THR:CA | 1:122:A:THR:C | 3                   | 1.61 | 0.53            | 1.45   |
| (1,165) | 1:84:A:GLY:C  | 1:85:A:TYR:N   | 1:85:A:TYR:CA  | 1:85:A:TYR:C  | 3                   | 1.37 | 0.26            | 1.42   |
| (1,136) | 1:110:A:ASP:N | 1:110:A:ASP:CA | 1:110:A:ASP:C  | 1:111:A:VAL:N | 3                   | 1.29 | 0.21            | 1.28   |
| (1,55)  | 1:53:A:ASP:C  | 1:54:A:ASN:N   | 1:54:A:ASN:CA  | 1:54:A:ASN:C  | 2                   | 1.82 | 0.73            | 1.82   |
| (1,53)  | 1:52:A:LEU:C  | 1:53:A:ASP:N   | 1:53:A:ASP:CA  | 1:53:A:ASP:C  | 2                   | 1.53 | 0.09            | 1.53   |
| (1,134) | 1:109:A:VAL:N | 1:109:A:VAL:CA | 1:109:A:VAL:C  | 1:110:A:ASP:N | 2                   | 1.34 | 0.28            | 1.34   |
| (1,73)  | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C   | 1:66:A:ALA:N  | 2                   | 1.16 | 0.06            | 1.16   |

<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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,92)  | 1:80:A:TYR:C  | 1:81:A:PRO:N   | 1:81:A:PRO:CA  | 1:81:A:PRO:C  | 8        | 6.23          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 2        | 5.1           |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 8        | 4.83          |
| (1,156) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C  | 1:125:A:ASP:N | 6        | 4.69          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 3        | 4.19          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 1        | 4.08          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 7        | 4.05          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 6        | 3.97          |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 3        | 3.74          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 10       | 3.6           |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 1        | 3.51          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 7        | 3.48          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 3        | 3.44          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 9        | 3.41          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 6        | 3.39          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 4        | 3.33          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 3        | 3.17          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 9        | 3.16          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 4        | 3.07          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 3        | 3.06          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 2        | 3.05          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 1        | 3.01          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 8        | 2.99          |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 7        | 2.95          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 10       | 2.95          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 8        | 2.93          |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1        | 2.9           |
| (1,173) | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C  | 1:118:A:GLY:N | 9        | 2.89          |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 3        | 2.89          |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 6        | 2.83          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 4        | 2.8           |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 2        | 2.79          |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 8        | 2.78          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 5        | 2.76          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 5        | 2.74          |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 9        | 2.73          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 9        | 2.73          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 2        | 2.7           |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 5        | 2.69          |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 9        | 2.68          |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 9        | 2.62          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 4        | 2.62          |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 3        | 2.62          |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 6        | 2.61          |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 10       | 2.61          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 7        | 2.57          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 6        | 2.57          |
| (1,55)  | 1:53:A:ASP:C  | 1:54:A:ASN:N   | 1:54:A:ASN:CA  | 1:54:A:ASN:C  | 9        | 2.55          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 4        | 2.54          |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 10       | 2.53          |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 4        | 2.49          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 5        | 2.49          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 4        | 2.48          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 1        | 2.44          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 9        | 2.38          |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 5        | 2.37          |
| (1,69)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:GLY:N  | 4        | 2.37          |
| (1,151) | 1:121:A:ASP:C | 1:122:A:THR:N  | 1:122:A:THR:CA | 1:122:A:THR:C | 10       | 2.33          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 6        | 2.33          |
| (1,101) | 1:86:A:ILE:C  | 1:87:A:ARG:N   | 1:87:A:ARG:CA  | 1:87:A:ARG:C  | 10       | 2.31          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 8        | 2.31          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 7        | 2.29          |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 4        | 2.29          |
| (1,57)  | 1:55:A:SER:N  | 1:55:A:SER:CA  | 1:55:A:SER:C   | 1:56:A:ARG:N  | 4        | 2.25          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 9        | 2.24          |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 2        | 2.21          |
| (1,173) | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C  | 1:118:A:GLY:N | 2        | 2.2           |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 6        | 2.17          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 2        | 2.16          |
| (1,81)  | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C   | 1:71:A:PRO:N  | 1        | 2.15          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 10       | 2.11          |
| (1,74)  | 1:65:A:GLY:C  | 1:66:A:ALA:N   | 1:66:A:ALA:CA  | 1:66:A:ALA:C  | 5        | 2.09          |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 2        | 2.08          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 5        | 1.98          |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 7        | 1.96          |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 10       | 1.95          |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 7        | 1.95          |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 1        | 1.91          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 9        | 1.88          |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 6        | 1.87          |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 6        | 1.85          |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 2        | 1.81          |
| (1,156) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C  | 1:125:A:ASP:N | 10       | 1.78          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 6        | 1.76          |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 8        | 1.75          |
| (1,79)  | 1:69:A:LYS:N  | 1:69:A:LYS:CA  | 1:69:A:LYS:C   | 1:70:A:LYS:N  | 6        | 1.74          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 5        | 1.72          |
| (1,2)   | 1:27:A:ASN:N  | 1:27:A:ASN:CA  | 1:27:A:ASN:C   | 1:28:A:LYS:N  | 5        | 1.72          |
| (1,85)  | 1:75:A:PRO:N  | 1:75:A:PRO:CA  | 1:75:A:PRO:C   | 1:76:A:GLU:N  | 8        | 1.67          |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 1        | 1.67          |
| (1,165) | 1:84:A:GLY:C  | 1:85:A:TYR:N   | 1:85:A:TYR:CA  | 1:85:A:TYR:C  | 1        | 1.66          |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 7        | 1.66          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 3        | 1.65          |
| (1,134) | 1:109:A:VAL:N | 1:109:A:VAL:CA | 1:109:A:VAL:C  | 1:110:A:ASP:N | 7        | 1.63          |
| (1,98)  | 1:83:A:ASP:C  | 1:84:A:GLY:N   | 1:84:A:GLY:CA  | 1:84:A:GLY:C  | 8        | 1.62          |
| (1,53)  | 1:52:A:LEU:C  | 1:53:A:ASP:N   | 1:53:A:ASP:CA  | 1:53:A:ASP:C  | 10       | 1.62          |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 5        | 1.62          |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 9        | 1.62          |
| (1,136) | 1:110:A:ASP:N | 1:110:A:ASP:CA | 1:110:A:ASP:C  | 1:111:A:VAL:N | 7        | 1.56          |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 1        | 1.55          |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 5        | 1.55          |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 7        | 1.55          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 1        | 1.53          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,81)  | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C   | 1:71:A:PRO:N  | 3        | 1.53          |
| (1,12)  | 1:32:A:ASP:N  | 1:32:A:ASP:CA  | 1:32:A:ASP:C   | 1:33:A:ARG:N  | 1        | 1.52          |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 2        | 1.51          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 1        | 1.5           |
| (1,108) | 1:90:A:PRO:N  | 1:90:A:PRO:CA  | 1:90:A:PRO:C   | 1:91:A:GLN:N  | 5        | 1.49          |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 8        | 1.49          |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 9        | 1.47          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 2        | 1.46          |
| (1,90)  | 1:79:A:SER:C  | 1:80:A:TYR:N   | 1:80:A:TYR:CA  | 1:80:A:TYR:C  | 9        | 1.46          |
| (1,151) | 1:121:A:ASP:C | 1:122:A:THR:N  | 1:122:A:THR:CA | 1:122:A:THR:C | 6        | 1.45          |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 10       | 1.45          |
| (1,53)  | 1:52:A:LEU:C  | 1:53:A:ASP:N   | 1:53:A:ASP:CA  | 1:53:A:ASP:C  | 7        | 1.44          |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 4        | 1.44          |
| (1,165) | 1:84:A:GLY:C  | 1:85:A:TYR:N   | 1:85:A:TYR:CA  | 1:85:A:TYR:C  | 6        | 1.42          |
| (1,7)   | 1:29:A:GLU:C  | 1:30:A:LYS:N   | 1:30:A:LYS:CA  | 1:30:A:LYS:C  | 1        | 1.41          |
| (1,173) | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C  | 1:118:A:GLY:N | 8        | 1.38          |
| (1,158) | 1:126:A:ILE:N | 1:126:A:ILE:CA | 1:126:A:ILE:C  | 1:127:A:GLY:N | 10       | 1.38          |
| (1,104) | 1:88:A:ARG:N  | 1:88:A:ARG:CA  | 1:88:A:ARG:C   | 1:89:A:LEU:N  | 2        | 1.38          |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 2        | 1.38          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 8        | 1.34          |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 3        | 1.32          |
| (1,96)  | 1:82:A:GLN:C  | 1:83:A:ASP:N   | 1:83:A:ASP:CA  | 1:83:A:ASP:C  | 2        | 1.31          |
| (1,156) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C  | 1:125:A:ASP:N | 1        | 1.3           |
| (1,136) | 1:110:A:ASP:N | 1:110:A:ASP:CA | 1:110:A:ASP:C  | 1:111:A:VAL:N | 10       | 1.28          |
| (1,13)  | 1:32:A:ASP:C  | 1:33:A:ARG:N   | 1:33:A:ARG:CA  | 1:33:A:ARG:C  | 6        | 1.28          |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 8        | 1.26          |
| (1,163) | 1:129:A:TRP:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 3        | 1.24          |
| (1,73)  | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C   | 1:66:A:ALA:N  | 1        | 1.23          |
| (1,99)  | 1:85:A:TYR:C  | 1:86:A:ILE:N   | 1:86:A:ILE:CA  | 1:86:A:ILE:C  | 1        | 1.22          |
| (1,97)  | 1:83:A:ASP:N  | 1:83:A:ASP:CA  | 1:83:A:ASP:C   | 1:84:A:GLY:N  | 3        | 1.22          |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 10       | 1.22          |
| (1,81)  | 1:70:A:LYS:N  | 1:70:A:LYS:CA  | 1:70:A:LYS:C   | 1:71:A:PRO:N  | 10       | 1.2           |
| (1,50)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA  | 1:51:A:LYS:C   | 1:52:A:LEU:N  | 9        | 1.18          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 2        | 1.17          |
| (1,164) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:VAL:N | 7        | 1.16          |
| (1,73)  | 1:65:A:GLY:N  | 1:65:A:GLY:CA  | 1:65:A:GLY:C   | 1:66:A:ALA:N  | 2        | 1.1           |
| (1,55)  | 1:53:A:ASP:C  | 1:54:A:ASN:N   | 1:54:A:ASN:CA  | 1:54:A:ASN:C  | 8        | 1.09          |
| (1,119) | 1:96:A:ALA:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 10       | 1.07          |
| (1,134) | 1:109:A:VAL:N | 1:109:A:VAL:CA | 1:109:A:VAL:C  | 1:110:A:ASP:N | 4        | 1.06          |
| (1,151) | 1:121:A:ASP:C | 1:122:A:THR:N  | 1:122:A:THR:CA | 1:122:A:THR:C | 2        | 1.05          |
| (1,165) | 1:84:A:GLY:C  | 1:85:A:TYR:N   | 1:85:A:TYR:CA  | 1:85:A:TYR:C  | 7        | 1.04          |
| (1,136) | 1:110:A:ASP:N | 1:110:A:ASP:CA | 1:110:A:ASP:C  | 1:111:A:VAL:N | 5        | 1.04          |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 7        | 1.03          |
| (1,117) | 1:95:A:GLY:C  | 1:96:A:ALA:N   | 1:96:A:ALA:CA  | 1:96:A:ALA:C  | 7        | 1.01          |
| (1,33)  | 1:42:A:ALA:C  | 1:43:A:LEU:N   | 1:43:A:LEU:CA  | 1:43:A:LEU:C  | 4        | 1.0           |