



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 12:45 AM UTC

PDB ID : 9RKK / pdb\_00009rkk  
BMRB ID : 34999  
Title : Staphylokinase Star WT  
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Deposited on : 2025-06-13

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

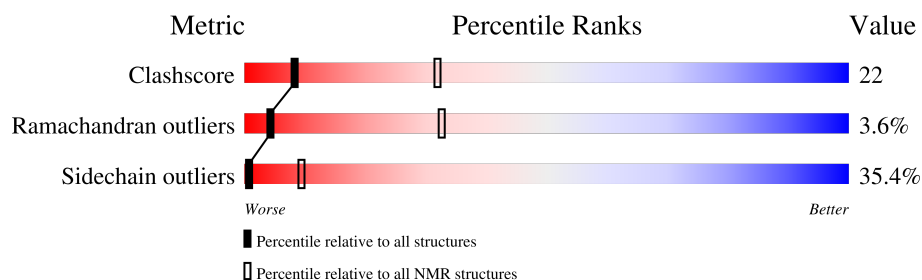
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 94%.

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     | 136    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:19-A:72, A:76-A:136<br>(115) | 0.20              | 19           |

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 4 clusters and 1 single-model cluster was found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2192 atoms, of which 1096 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Staphylokinase.

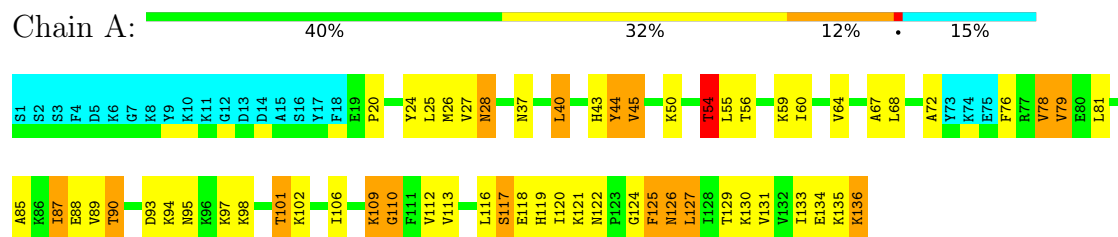
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 136      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2192  | 713 | 1096 | 169 | 213 | 1 |       |

## 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: Staphylokinase

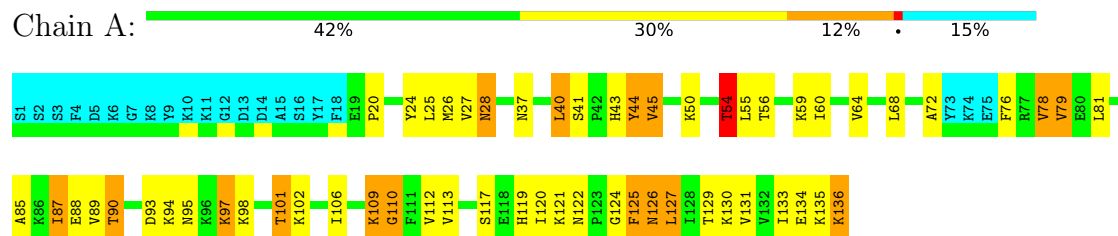


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

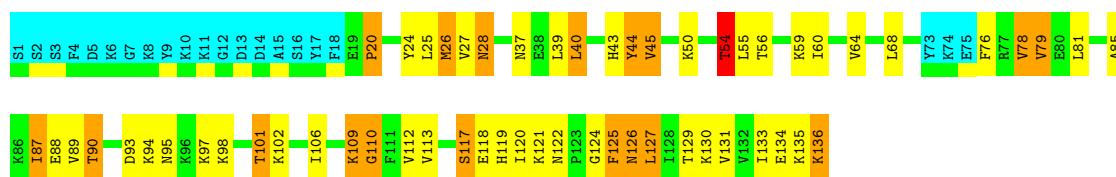
- Molecule 1: Staphylokinase



#### 4.2.2 Score per residue for model 2

- Molecule 1: Staphylokinase

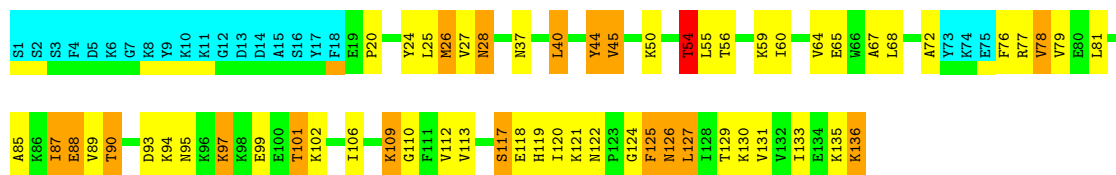




### 4.2.3 Score per residue for model 3

- Molecule 1: Staphylokinase

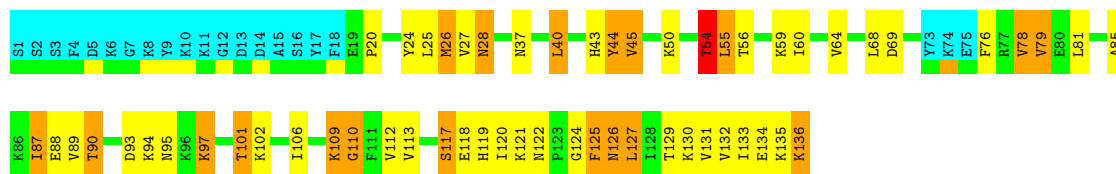
Chain A: 41% 30% 12% 15%



### 4.2.4 Score per residue for model 4

- Molecule 1: Staphylokinase

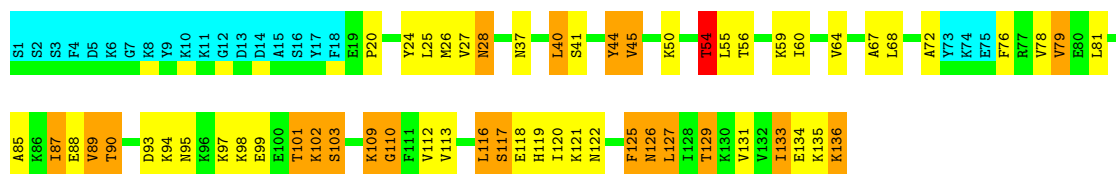
Chain A: 42% 28% 14% 15%



### 4.2.5 Score per residue for model 5

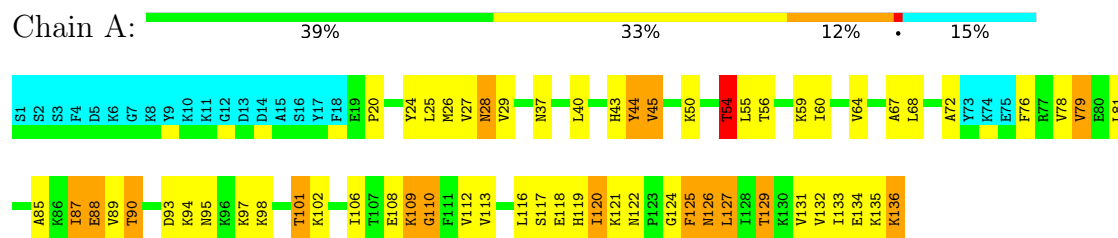
- Molecule 1: Staphylokinase

Chain A: 41% 27% 15% 15%



### 4.2.6 Score per residue for model 6

- Molecule 1: Staphylokinase



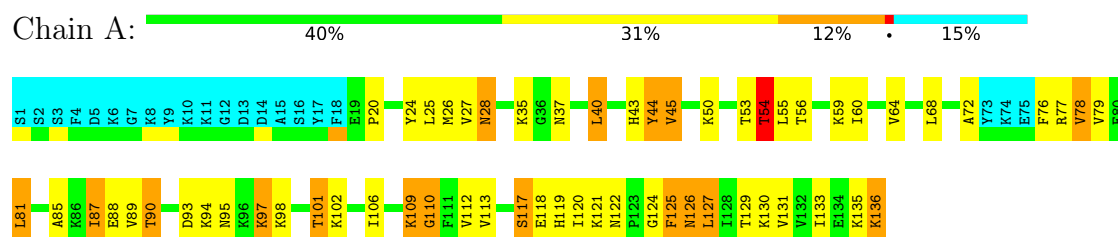
#### 4.2.7 Score per residue for model 7

- Molecule 1: Staphylokinase



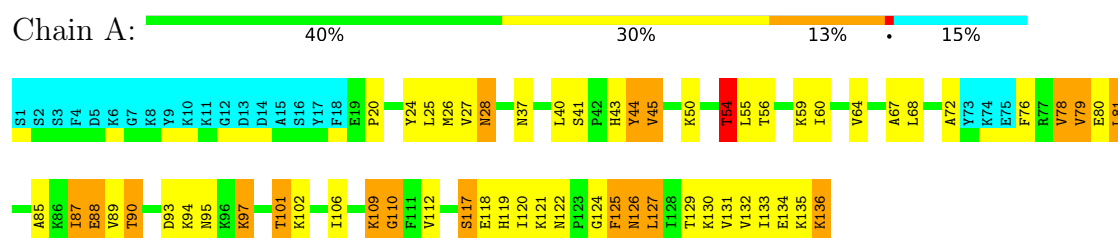
#### 4.2.8 Score per residue for model 8

- Molecule 1: Staphylokinase



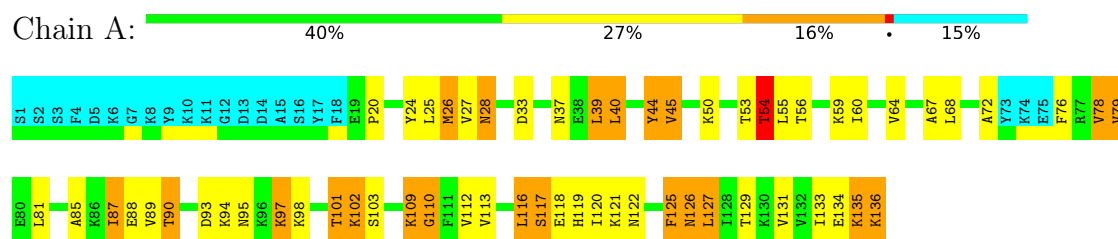
#### 4.2.9 Score per residue for model 9

- Molecule 1: Staphylokinase



#### 4.2.10 Score per residue for model 10

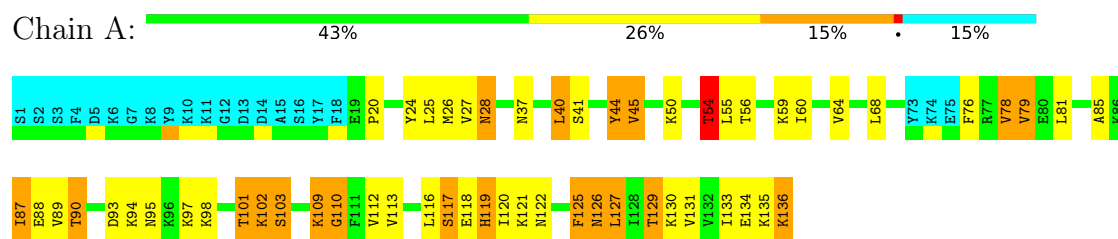
- Molecule 1: Staphylokinase





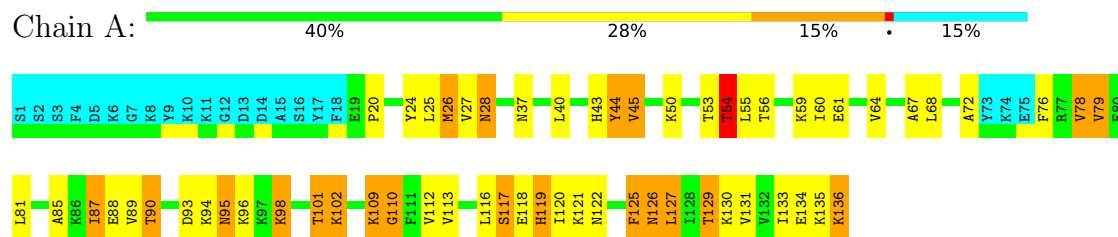
### 4.2.14 Score per residue for model 14

- Molecule 1: Staphylokinase



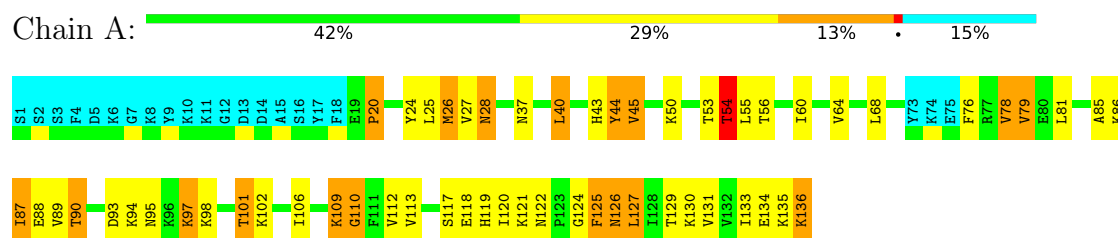
### 4.2.18 Score per residue for model 18

- Molecule 1: Staphylokinase



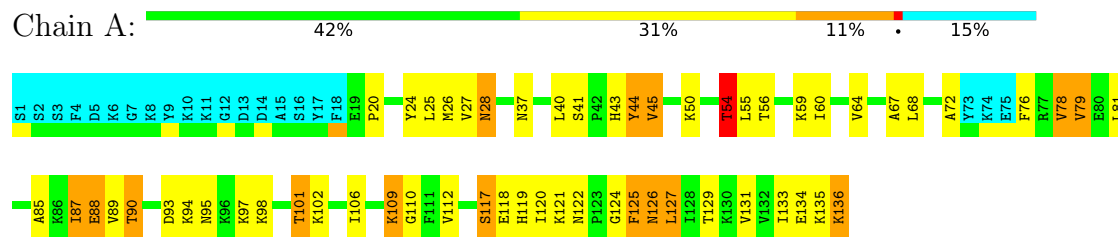
### 4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: Staphylokinase



### 4.2.20 Score per residue for model 20

- Molecule 1: Staphylokinase



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CYANA         | structure calculation |         |
| ARTINA        | 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                       | 1737           |
| Number of shifts mapped to atoms             | 1737           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 94%            |

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 923   | 937      | 937      | 40±2    |
| All | All   | 18460 | 18740    | 18740    | 806     |

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:25:LEU:HD11 | 1:A:127:LEU:HD21 | 0.81     | 1.52        | 20     | 20    |
| 1:A:85:ALA:HB2  | 1:A:129:THR:HG21 | 0.71     | 1.59        | 7      | 20    |
| 1:A:26:MET:HE3  | 1:A:126:ASN:HB3  | 0.70     | 1.62        | 1      | 8     |
| 1:A:90:THR:HG23 | 1:A:101:THR:OG1  | 0.70     | 1.86        | 16     | 20    |
| 1:A:26:MET:HE2  | 1:A:126:ASN:HB3  | 0.66     | 1.67        | 15     | 3     |
| 1:A:68:LEU:C    | 1:A:68:LEU:HD12  | 0.64     | 2.17        | 7      | 20    |
| 1:A:27:VAL:O    | 1:A:27:VAL:HG13  | 0.63     | 1.94        | 3      | 20    |
| 1:A:85:ALA:HB2  | 1:A:129:THR:CG2  | 0.63     | 2.23        | 7      | 20    |
| 1:A:109:LYS:N   | 1:A:109:LYS:HD3  | 0.62     | 2.09        | 19     | 1     |
| 1:A:88:GLU:HA   | 1:A:102:LYS:O    | 0.62     | 1.95        | 3      | 19    |
| 1:A:44:TYR:CD2  | 1:A:44:TYR:C     | 0.61     | 2.79        | 18     | 20    |
| 1:A:68:LEU:CD2  | 1:A:78:VAL:HG23  | 0.60     | 2.26        | 3      | 11    |
| 1:A:72:ALA:HB1  | 1:A:76:PHE:CD1   | 0.59     | 2.32        | 16     | 10    |
| 1:A:87:ILE:CG1  | 1:A:106:ILE:HD11 | 0.59     | 2.28        | 8      | 13    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:40:LEU:HD23  | 1:A:76:PHE:CE1   | 0.58     | 2.33        | 10     | 11    |
| 1:A:55:LEU:HD21  | 1:A:87:ILE:HD11  | 0.58     | 1.76        | 1      | 12    |
| 1:A:87:ILE:HG13  | 1:A:106:ILE:HD11 | 0.56     | 1.77        | 7      | 12    |
| 1:A:40:LEU:HD21  | 1:A:72:ALA:HA    | 0.56     | 1.76        | 5      | 4     |
| 1:A:60:ILE:HG13  | 1:A:106:ILE:HG21 | 0.55     | 1.78        | 9      | 4     |
| 1:A:68:LEU:HD22  | 1:A:78:VAL:HG23  | 0.55     | 1.77        | 1      | 18    |
| 1:A:79:VAL:HG13  | 1:A:134:GLU:HB3  | 0.54     | 1.80        | 9      | 16    |
| 1:A:60:ILE:O     | 1:A:64:VAL:HG22  | 0.53     | 2.03        | 8      | 19    |
| 1:A:113:VAL:HG13 | 1:A:125:PHE:CE2  | 0.53     | 2.38        | 14     | 16    |
| 1:A:25:LEU:CD1   | 1:A:127:LEU:HD21 | 0.53     | 2.32        | 20     | 20    |
| 1:A:126:ASN:C    | 1:A:127:LEU:HD13 | 0.52     | 2.28        | 16     | 20    |
| 1:A:135:LYS:O    | 1:A:136:LYS:C    | 0.51     | 2.53        | 7      | 20    |
| 1:A:25:LEU:C     | 1:A:25:LEU:HD13  | 0.51     | 2.31        | 9      | 20    |
| 1:A:27:VAL:HG11  | 1:A:67:ALA:CB    | 0.51     | 2.35        | 20     | 11    |
| 1:A:125:PHE:CD1  | 1:A:125:PHE:N    | 0.50     | 2.79        | 4      | 20    |
| 1:A:127:LEU:N    | 1:A:127:LEU:HD13 | 0.50     | 2.21        | 20     | 3     |
| 1:A:87:ILE:O     | 1:A:103:SER:HA   | 0.50     | 2.06        | 5      | 4     |
| 1:A:54:THR:N     | 1:A:112:VAL:HG12 | 0.50     | 2.21        | 18     | 20    |
| 1:A:25:LEU:HD11  | 1:A:127:LEU:CD2  | 0.50     | 2.34        | 18     | 14    |
| 1:A:27:VAL:O     | 1:A:27:VAL:CG1   | 0.50     | 2.59        | 18     | 19    |
| 1:A:55:LEU:HD23  | 1:A:55:LEU:C     | 0.49     | 2.33        | 10     | 8     |
| 1:A:90:THR:HG21  | 1:A:99:GLU:OE1   | 0.49     | 2.07        | 5      | 3     |
| 1:A:26:MET:O     | 1:A:127:LEU:HD22 | 0.48     | 2.08        | 13     | 6     |
| 1:A:127:LEU:HD13 | 1:A:127:LEU:N    | 0.48     | 2.22        | 7      | 17    |
| 1:A:87:ILE:HG23  | 1:A:125:PHE:HB3  | 0.48     | 1.83        | 3      | 20    |
| 1:A:45:VAL:HG21  | 1:A:67:ALA:HB1   | 0.48     | 1.85        | 18     | 10    |
| 1:A:27:VAL:HG12  | 1:A:45:VAL:HB    | 0.47     | 1.86        | 1      | 20    |
| 1:A:127:LEU:HD22 | 1:A:127:LEU:H    | 0.47     | 1.70        | 3      | 20    |
| 1:A:54:THR:CA    | 1:A:112:VAL:HG12 | 0.47     | 2.40        | 5      | 20    |
| 1:A:60:ILE:O     | 1:A:64:VAL:HG13  | 0.47     | 2.10        | 5      | 14    |
| 1:A:28:ASN:O     | 1:A:127:LEU:O    | 0.47     | 2.32        | 9      | 20    |
| 1:A:90:THR:OG1   | 1:A:101:THR:HG23 | 0.47     | 2.10        | 5      | 18    |
| 1:A:89:VAL:HG13  | 1:A:102:LYS:NZ   | 0.46     | 2.24        | 16     | 2     |
| 1:A:68:LEU:C     | 1:A:68:LEU:CD1   | 0.46     | 2.88        | 7      | 7     |
| 1:A:87:ILE:O     | 1:A:87:ILE:HG22  | 0.46     | 2.09        | 5      | 7     |
| 1:A:127:LEU:N    | 1:A:127:LEU:HD22 | 0.46     | 2.25        | 18     | 12    |
| 1:A:127:LEU:HD22 | 1:A:127:LEU:N    | 0.46     | 2.26        | 5      | 8     |
| 1:A:89:VAL:HG23  | 1:A:124:GLY:O    | 0.45     | 2.11        | 20     | 13    |
| 1:A:40:LEU:HB2   | 1:A:133:ILE:HD12 | 0.45     | 1.87        | 5      | 1     |
| 1:A:109:LYS:O    | 1:A:110:GLY:C    | 0.45     | 2.59        | 4      | 20    |
| 1:A:64:VAL:HG21  | 1:A:81:LEU:HD23  | 0.45     | 1.89        | 8      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:40:LEU:HD11 | 1:A:71:THR:HG22  | 0.45     | 1.89        | 15     | 1     |
| 1:A:116:LEU:HB3 | 1:A:120:ILE:HG23 | 0.45     | 1.88        | 5      | 10    |
| 1:A:44:TYR:C    | 1:A:45:VAL:CG2   | 0.44     | 2.91        | 9      | 20    |
| 1:A:93:ASP:HA   | 1:A:119:HIS:CD2  | 0.43     | 2.49        | 14     | 3     |
| 1:A:53:THR:O    | 1:A:112:VAL:HA   | 0.42     | 2.14        | 10     | 6     |
| 1:A:25:LEU:HD21 | 1:A:127:LEU:HD11 | 0.42     | 1.91        | 13     | 2     |
| 1:A:93:ASP:HB2  | 1:A:95:ASN:ND2   | 0.42     | 2.30        | 18     | 1     |
| 1:A:93:ASP:O    | 1:A:97:LYS:N     | 0.41     | 2.54        | 5      | 16    |
| 1:A:79:VAL:CG2  | 1:A:132:VAL:HG12 | 0.41     | 2.46        | 9      | 1     |
| 1:A:80:GLU:C    | 1:A:81:LEU:HD23  | 0.41     | 2.40        | 9      | 1     |
| 1:A:93:ASP:CG   | 1:A:98:LYS:O     | 0.41     | 2.63        | 15     | 2     |
| 1:A:33:ASP:CG   | 1:A:39:LEU:HD12  | 0.41     | 2.41        | 15     | 3     |
| 1:A:68:LEU:HD12 | 1:A:69:ASP:N     | 0.41     | 2.31        | 4      | 1     |
| 1:A:27:VAL:HG11 | 1:A:67:ALA:HB2   | 0.41     | 1.92        | 10     | 1     |
| 1:A:29:VAL:HA   | 1:A:129:THR:O    | 0.41     | 2.16        | 6      | 1     |
| 1:A:55:LEU:HD21 | 1:A:87:ILE:CD1   | 0.40     | 2.47        | 14     | 1     |
| 1:A:77:ARG:HB3  | 1:A:136:LYS:N    | 0.40     | 2.32        | 3      | 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     | 114/136 (84%)   | 95±2 (83±2%) | 15±2 (13±2%) | 4±0 (4±0%) | 4           | 32 |
| All | All   | 2280/2720 (84%) | 1899 (83%)   | 300 (13%)    | 81 (4%)    | 4           | 32 |

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 20  | PRO  | 20             |
| 1   | A     | 54  | THR  | 20             |
| 1   | A     | 117 | SER  | 20             |
| 1   | A     | 110 | GLY  | 18             |
| 1   | A     | 72  | ALA  | 3              |

### 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     | 105/123 (85%)   | 68±2 (65±2%) | 37±2 (35±2%) | 1 9         |
| All | All   | 2100/2460 (85%) | 1356 (65%)   | 744 (35%)    | 1 9         |

All 56 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     | 24  | TYR  | 20             |
| 1   | A     | 28  | ASN  | 20             |
| 1   | A     | 37  | ASN  | 20             |
| 1   | A     | 40  | LEU  | 20             |
| 1   | A     | 44  | TYR  | 20             |
| 1   | A     | 45  | VAL  | 20             |
| 1   | A     | 50  | LYS  | 20             |
| 1   | A     | 54  | THR  | 20             |
| 1   | A     | 56  | THR  | 20             |
| 1   | A     | 78  | VAL  | 20             |
| 1   | A     | 79  | VAL  | 20             |
| 1   | A     | 81  | LEU  | 20             |
| 1   | A     | 87  | ILE  | 20             |
| 1   | A     | 90  | THR  | 20             |
| 1   | A     | 94  | LYS  | 20             |
| 1   | A     | 95  | ASN  | 20             |
| 1   | A     | 101 | THR  | 20             |
| 1   | A     | 109 | LYS  | 20             |
| 1   | A     | 119 | HIS  | 20             |
| 1   | A     | 122 | ASN  | 20             |
| 1   | A     | 125 | PHE  | 20             |
| 1   | A     | 126 | ASN  | 20             |
| 1   | A     | 127 | LEU  | 20             |
| 1   | A     | 131 | VAL  | 20             |
| 1   | A     | 133 | ILE  | 20             |
| 1   | A     | 136 | LYS  | 20             |
| 1   | A     | 59  | LYS  | 19             |
| 1   | A     | 121 | LYS  | 19             |
| 1   | A     | 118 | GLU  | 19             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 43  | HIS  | 15             |
| 1   | A     | 130 | LYS  | 14             |
| 1   | A     | 117 | SER  | 14             |
| 1   | A     | 97  | LYS  | 13             |
| 1   | A     | 120 | ILE  | 13             |
| 1   | A     | 98  | LYS  | 12             |
| 1   | A     | 26  | MET  | 12             |
| 1   | A     | 41  | SER  | 10             |
| 1   | A     | 88  | GLU  | 8              |
| 1   | A     | 89  | VAL  | 7              |
| 1   | A     | 102 | LYS  | 7              |
| 1   | A     | 129 | THR  | 7              |
| 1   | A     | 103 | SER  | 5              |
| 1   | A     | 116 | LEU  | 5              |
| 1   | A     | 108 | GLU  | 4              |
| 1   | A     | 39  | LEU  | 3              |
| 1   | A     | 132 | VAL  | 3              |
| 1   | A     | 35  | LYS  | 2              |
| 1   | A     | 86  | LYS  | 2              |
| 1   | A     | 77  | ARG  | 2              |
| 1   | A     | 135 | LYS  | 2              |
| 1   | A     | 61  | GLU  | 2              |
| 1   | A     | 65  | GLU  | 1              |
| 1   | A     | 55  | LEU  | 1              |
| 1   | A     | 76  | PHE  | 1              |
| 1   | A     | 82  | ASP  | 1              |
| 1   | A     | 96  | LYS  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 93% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

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

|   |      |
|---|------|
| Total number of shifts                  | 1737 |
| Number of shifts mapped to atoms        | 1737 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 14   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 136      | $2.78 \pm 0.10$                 | Should be applied          |
| $^{13}\text{C}_\beta$  | 128      | $2.68 \pm 0.10$                 | Should be applied          |
| $^{13}\text{C}'$       | 122      | $2.96 \pm 0.12$                 | Should be applied          |
| $^{15}\text{N}$        | 126      | $-0.48 \pm 0.25$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1493 atoms were assigned a chemical shift out of a possible 1591. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 549/563 (98%) | 227/227 (100%) | 216/230 (94%)   | 106/106 (100%)  |
| Sidechain | 852/898 (95%) | 579/583 (99%)  | 268/292 (92%)   | 5/23 (22%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 92/130 (71%)    | 59/63 (94%)    | 32/64 (50%)     | 1/3 (33%)       |
| Overall  | 1493/1591 (94%) | 865/873 (99%)  | 516/586 (88%)   | 112/132 (85%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1737 atoms were assigned a chemical shift out of a possible 1860. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 654/670 (98%)   | 270/271 (100%)  | 258/272 (95%)   | 126/127 (99%)   |
| Sidechain | 958/1013 (95%)  | 650/654 (99%)   | 303/331 (92%)   | 5/28 (18%)      |
| Aromatic  | 125/177 (71%)   | 81/85 (95%)     | 43/89 (48%)     | 1/3 (33%)       |
| Overall   | 1737/1860 (93%) | 1001/1010 (99%) | 604/692 (87%)   | 132/158 (84%)   |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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.

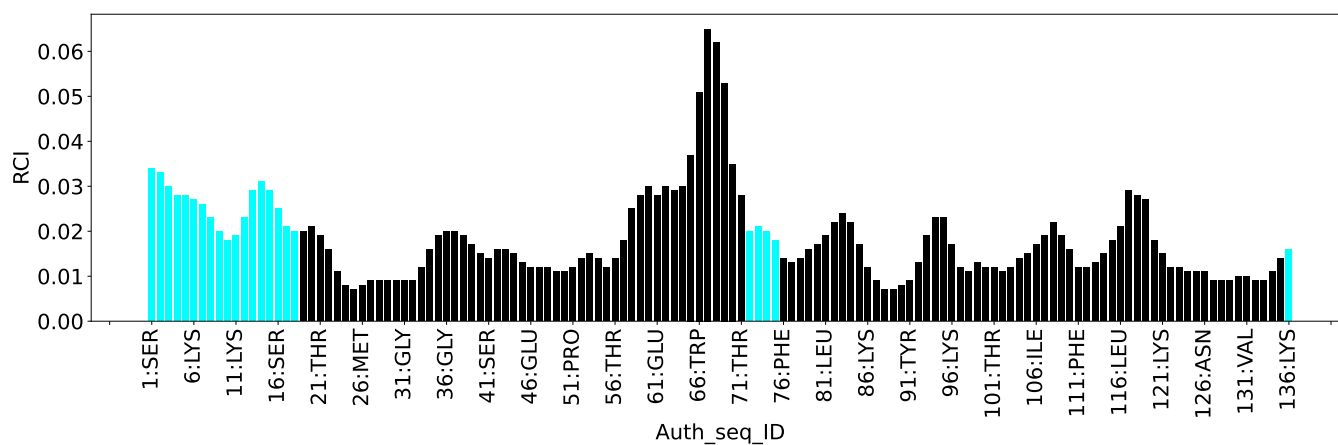
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 98  | LYS  | HD3  | 3.79       | 0.54 – 2.65         | 10.4    |
| 1       | A     | 102 | LYS  | HD3  | 3.62       | 0.54 – 2.65         | 9.6     |
| 1       | A     | 109 | LYS  | HE3  | 4.70       | 1.92 – 3.89         | 9.1     |
| 1       | A     | 86  | LYS  | HE3  | 4.70       | 1.92 – 3.89         | 9.1     |
| 1       | A     | 97  | LYS  | HE3  | 4.69       | 1.92 – 3.89         | 9.1     |
| 1       | A     | 104 | PHE  | HD1  | 4.70       | 5.51 – 8.60         | -7.6    |
| 1       | A     | 130 | LYS  | HE2  | 1.51       | 1.95 – 3.88         | -7.2    |
| 1       | A     | 59  | LYS  | HE2  | 1.51       | 1.95 – 3.88         | -7.2    |
| 1       | A     | 50  | LYS  | HB2  | 0.27       | 0.58 – 2.97         | -6.3    |
| 1       | A     | 130 | LYS  | HD2  | 2.85       | 0.58 – 2.64         | 6.1     |
| 1       | A     | 130 | LYS  | HD3  | 2.85       | 0.54 – 2.65         | 6.0     |
| 1       | A     | 59  | LYS  | HD3  | 2.81       | 0.54 – 2.65         | 5.7     |
| 1       | A     | 100 | GLU  | HB2  | 0.95       | 1.00 – 3.05         | -5.2    |
| 1       | A     | 75  | GLU  | HB2  | 0.97       | 1.00 – 3.05         | -5.1    |

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description  | Value |
|--|-------|
| Total distance restraints                                | 2159  |
| Intra-residue ( $ i-j =0$ )                              | 533   |
| Sequential ( $ i-j =1$ )                                 | 631   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 289   |
| Long range ( $ i-j \geq 5$ )                             | 706   |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 15.9  |
| Number of long range restraints per residue <sup>1</sup> | 5.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small)  | 35.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 21.8                                   | 0.5     |
| >0.5 (Large)     | 2.5                                    | 2.32    |

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

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

## 9 Distance violation analysis ⓘ

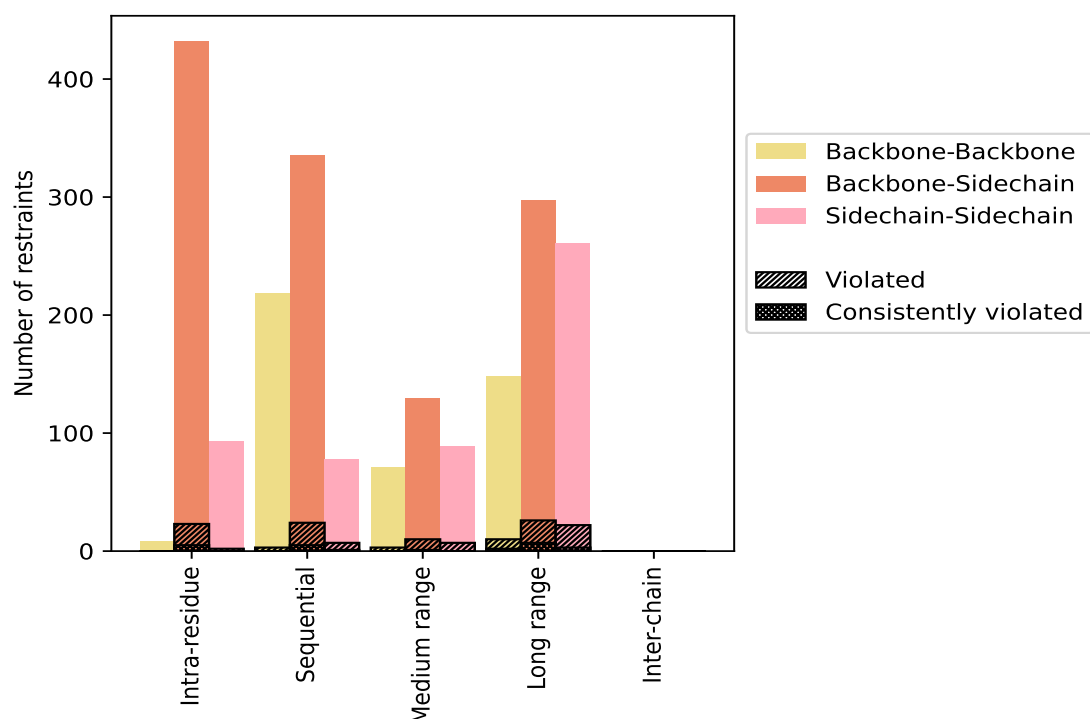
### 9.1 Summary of distance violations ⓘ

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

| Restrains type  | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|   |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>533</b>  | <b>24.7</b>    | <b>25</b>             | <b>4.7</b>     | <b>1.2</b>     | <b>5</b>                           | <b>0.9</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 8           | 0.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 432         | 20.0           | 23                    | 5.3            | 1.1            | 5                                  | 1.2            | 0.2            |
| Sidechain-Sidechain   | 93          | 4.3            | 2                     | 2.2            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>631</b>  | <b>29.2</b>    | <b>34</b>             | <b>5.4</b>     | <b>1.6</b>     | <b>6</b>                           | <b>1.0</b>     | <b>0.3</b>     |
| Backbone-Backbone   | 218         | 10.1           | 3                     | 1.4            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 335         | 15.5           | 24                    | 7.2            | 1.1            | 5                                  | 1.5            | 0.2            |
| Sidechain-Sidechain   | 78          | 3.6            | 7                     | 9.0            | 0.3            | 1                                  | 1.3            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>289</b>  | <b>13.4</b>    | <b>20</b>             | <b>6.9</b>     | <b>0.9</b>     | <b>1</b>                           | <b>0.3</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 71          | 3.3            | 3                     | 4.2            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 129         | 6.0            | 10                    | 7.8            | 0.5            | 1                                  | 0.8            | 0.0            |
| Sidechain-Sidechain   | 89          | 4.1            | 7                     | 7.9            | 0.3            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>706</b>  | <b>32.7</b>    | <b>58</b>             | <b>8.2</b>     | <b>2.7</b>     | <b>12</b>                          | <b>1.7</b>     | <b>0.6</b>     |
| Backbone-Backbone   | 148         | 6.9            | 10                    | 6.8            | 0.5            | 2                                  | 1.4            | 0.1            |
| Backbone-Sidechain  | 297         | 13.8           | 26                    | 8.8            | 1.2            | 7                                  | 2.4            | 0.3            |
| Sidechain-Sidechain   | 261         | 12.1           | 22                    | 8.4            | 1.0            | 3                                  | 1.1            | 0.1            |
| <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>2159</b> | <b>100.0</b>   | <b>137</b>            | <b>6.3</b>     | <b>6.3</b>     | <b>24</b>                          | <b>1.1</b>     | <b>1.1</b>     |
| Backbone-Backbone   | 445         | 20.6           | 16                    | 3.6            | 0.7            | 2                                  | 0.4            | 0.1            |
| Backbone-Sidechain  | 1193        | 55.3           | 83                    | 7.0            | 3.8            | 18                                 | 1.5            | 0.8            |
| Sidechain-Sidechain   | 521         | 24.1           | 38                    | 7.3            | 1.8            | 4                                  | 0.8            | 0.2            |

<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        | 11                   | 17              | 8               | 33              | 0               | 69    | 0.21     | 0.81    | 0.13                | 0.16       |
| 2        | 10                   | 14              | 5               | 31              | 0               | 60    | 0.21     | 0.81    | 0.13                | 0.18       |
| 3        | 12                   | 12              | 9               | 30              | 0               | 63    | 0.24     | 1.47    | 0.2                 | 0.19       |
| 4        | 12                   | 18              | 8               | 30              | 0               | 68    | 0.21     | 0.81    | 0.13                | 0.17       |
| 5        | 8                    | 14              | 8               | 28              | 0               | 58    | 0.21     | 0.81    | 0.13                | 0.18       |
| 6        | 11                   | 19              | 9               | 37              | 0               | 76    | 0.21     | 0.81    | 0.13                | 0.16       |
| 7        | 9                    | 15              | 7               | 34              | 0               | 65    | 0.21     | 0.81    | 0.13                | 0.16       |
| 8        | 10                   | 15              | 9               | 30              | 0               | 64    | 0.21     | 0.82    | 0.13                | 0.16       |
| 9        | 9                    | 18              | 10              | 37              | 0               | 74    | 0.22     | 0.81    | 0.13                | 0.18       |
| 10       | 9                    | 14              | 9               | 22              | 0               | 54    | 0.25     | 1.45    | 0.22                | 0.18       |

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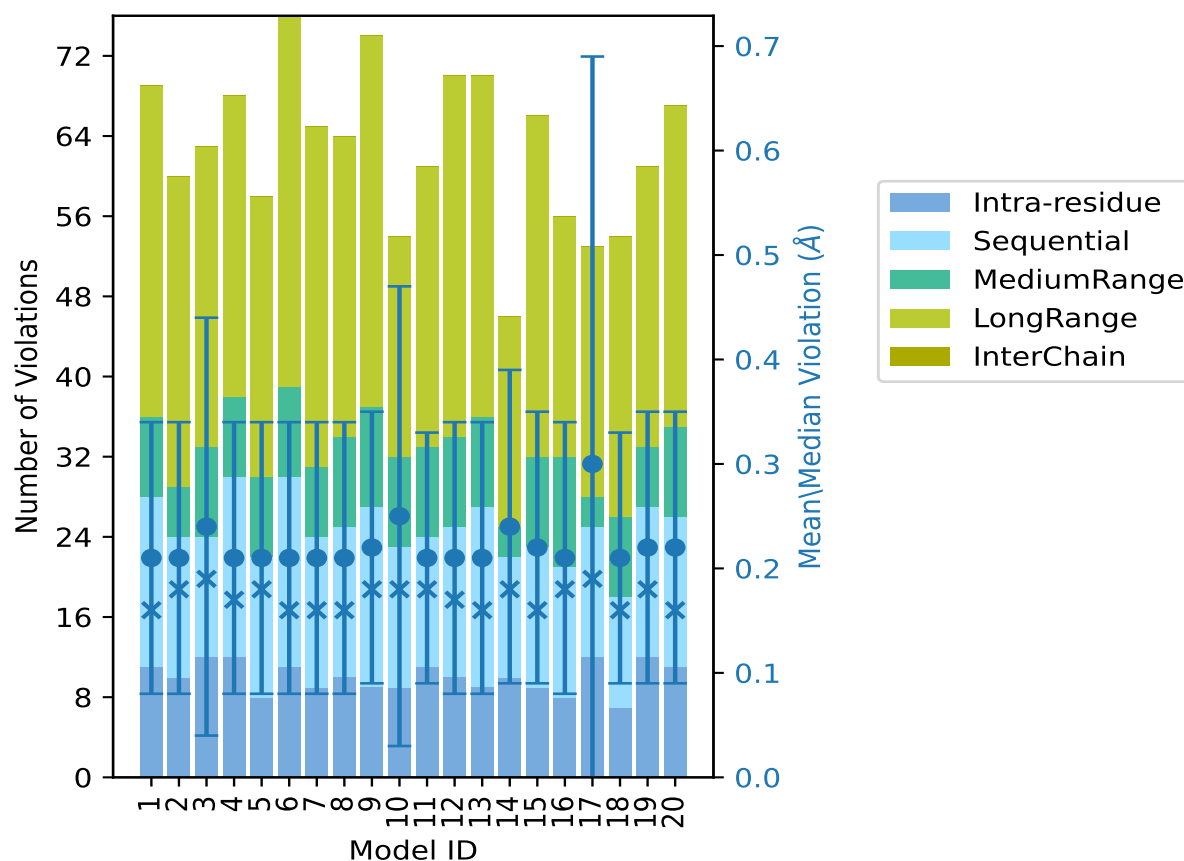
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 11                   | 13              | 9               | 28              | 0               | 61    | 0.21     | 0.81    | 0.12                | 0.18       |
| 12       | 10                   | 15              | 9               | 36              | 0               | 70    | 0.21     | 0.81    | 0.13                | 0.17       |
| 13       | 9                    | 18              | 9               | 34              | 0               | 70    | 0.21     | 0.81    | 0.13                | 0.16       |
| 14       | 10                   | 12              | 3               | 21              | 0               | 46    | 0.24     | 0.82    | 0.15                | 0.18       |
| 15       | 9                    | 14              | 9               | 34              | 0               | 66    | 0.22     | 0.81    | 0.13                | 0.16       |
| 16       | 8                    | 13              | 11              | 24              | 0               | 56    | 0.21     | 0.82    | 0.13                | 0.18       |
| 17       | 12                   | 13              | 3               | 25              | 0               | 53    | 0.3      | 2.32    | 0.39                | 0.19       |
| 18       | 7                    | 11              | 8               | 28              | 0               | 54    | 0.21     | 0.81    | 0.12                | 0.16       |
| 19       | 12                   | 15              | 6               | 28              | 0               | 61    | 0.22     | 0.81    | 0.13                | 0.18       |
| 20       | 11                   | 15              | 9               | 32              | 0               | 67    | 0.22     | 0.81    | 0.13                | 0.16       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

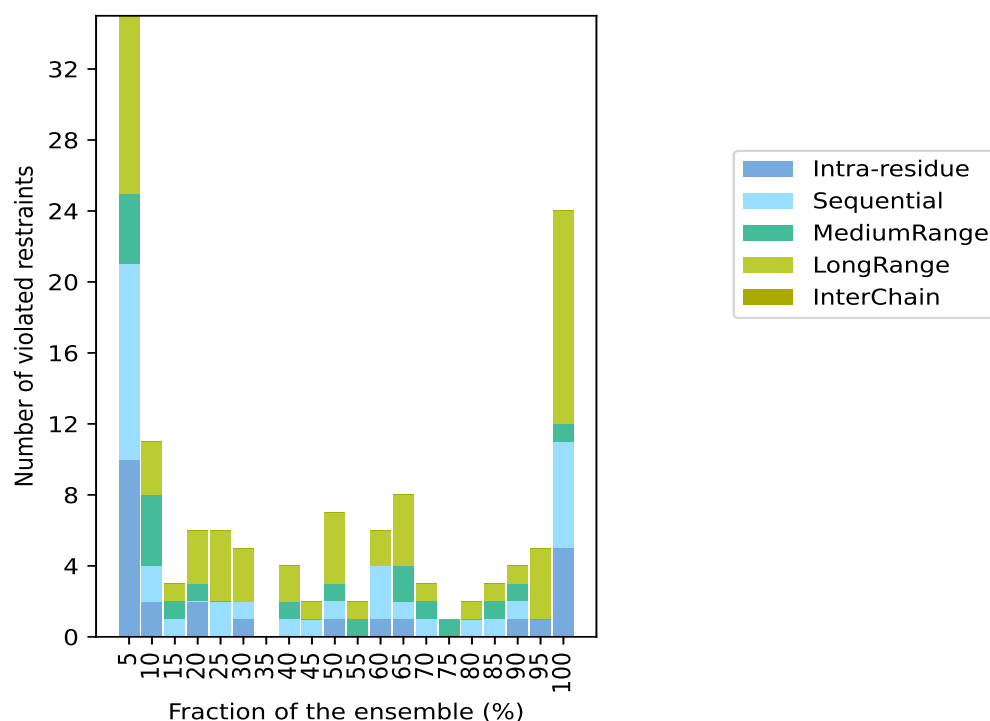
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2022(IR:508, SQ:597, MR:269, LR:648, IC:0) restraints are 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>       | %     |
| 10                            | 11              | 4               | 10              | 0               | 35    | 1                        | 5.0   |
| 2                             | 2               | 4               | 3               | 0               | 11    | 2                        | 10.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 3                        | 15.0  |
| 2                             | 0               | 1               | 3               | 0               | 6     | 4                        | 20.0  |
| 0                             | 2               | 0               | 4               | 0               | 6     | 5                        | 25.0  |
| 1                             | 1               | 0               | 3               | 0               | 5     | 6                        | 30.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 7                        | 35.0  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 8                        | 40.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 9                        | 45.0  |
| 1                             | 1               | 1               | 4               | 0               | 7     | 10                       | 50.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 11                       | 55.0  |
| 1                             | 3               | 0               | 2               | 0               | 6     | 12                       | 60.0  |
| 1                             | 1               | 2               | 4               | 0               | 8     | 13                       | 65.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 14                       | 70.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 15                       | 75.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 16                       | 80.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 17                       | 85.0  |
| 1                             | 1               | 1               | 1               | 0               | 4     | 18                       | 90.0  |
| 1                             | 0               | 0               | 4               | 0               | 5     | 19                       | 95.0  |
| 5                             | 6               | 1               | 12              | 0               | 24    | 20                       | 100.0 |

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

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

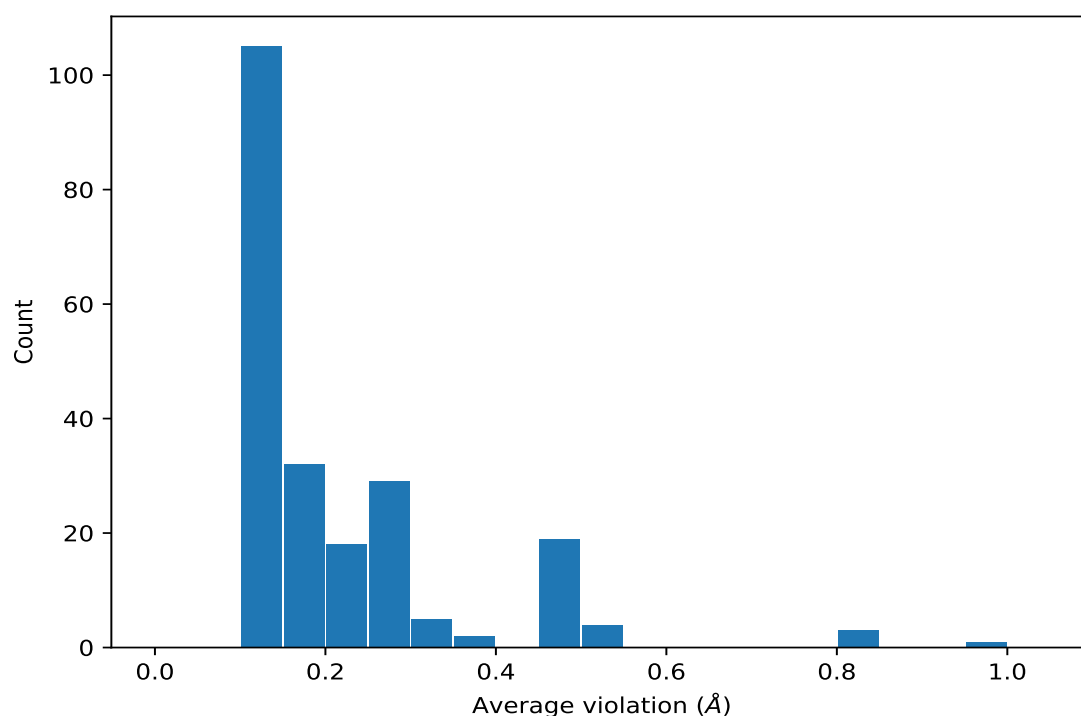
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,258)  | 1:45:A:VAL:HG21 | 1:46:A:GLU:H     | 20                  | 0.81     | 0.0                 | 0.81       |
| (1,258)  | 1:45:A:VAL:HG22 | 1:46:A:GLU:H     | 20                  | 0.81     | 0.0                 | 0.81       |
| (1,258)  | 1:45:A:VAL:HG23 | 1:46:A:GLU:H     | 20                  | 0.81     | 0.0                 | 0.81       |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 20                  | 0.51     | 0.01                | 0.51       |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 20                  | 0.51     | 0.01                | 0.51       |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 20                  | 0.51     | 0.01                | 0.51       |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 20                  | 0.45     | 0.01                | 0.45       |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 20                  | 0.45     | 0.01                | 0.45       |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 20                  | 0.45     | 0.01                | 0.45       |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H     | 20                  | 0.37     | 0.01                | 0.37       |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H     | 20                  | 0.36     | 0.01                | 0.36       |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 20                  | 0.31     | 0.04                | 0.31       |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 20                  | 0.31     | 0.04                | 0.31       |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 20                  | 0.3      | 0.01                | 0.3        |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 20                  | 0.28     | 0.01                | 0.28       |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 20                  | 0.26     | 0.06                | 0.28       |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 20                  | 0.26     | 0.02                | 0.26       |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 20                  | 0.26     | 0.04                | 0.26       |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 20                  | 0.26     | 0.04                | 0.26       |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 20                  | 0.26     | 0.04                | 0.26       |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 20                  | 0.26     | 0.04                | 0.26       |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 20                  | 0.26     | 0.04                | 0.26       |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 20                  | 0.26     | 0.04                | 0.26       |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 20                  | 0.25     | 0.03                | 0.24       |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 20                  | 0.23     | 0.01                | 0.23       |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 20                  | 0.23     | 0.01                | 0.23       |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 20                  | 0.23     | 0.01                | 0.23       |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 20                  | 0.23     | 0.01                | 0.23       |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 20                  | 0.23     | 0.01                | 0.23       |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 20                  | 0.23     | 0.01                | 0.23       |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 20                  | 0.23     | 0.03                | 0.22       |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 20                  | 0.23     | 0.03                | 0.22       |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 20                  | 0.22     | 0.03                | 0.22       |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 20                  | 0.22     | 0.05                | 0.21       |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 20                  | 0.22     | 0.05                | 0.21       |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 20                  | 0.22     | 0.05                | 0.21       |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 20                  | 0.21     | 0.04                | 0.2        |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 20                  | 0.2      | 0.03                | 0.19       |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 20                  | 0.19     | 0.01                | 0.2        |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 20                  | 0.19     | 0.01                | 0.19       |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 20                  | 0.18     | 0.03                | 0.18       |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 20                  | 0.15     | 0.02                | 0.16       |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 20                  | 0.12     | 0.02                | 0.11       |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 19                  | 0.29     | 0.05                | 0.32       |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 19                  | 0.29     | 0.05                | 0.32       |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 19                  | 0.27     | 0.14                | 0.21       |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 19                  | 0.27     | 0.14                | 0.21       |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 19                  | 0.27     | 0.14                | 0.21       |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 19                  | 0.16     | 0.03                | 0.16       |
| (1,483)  | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 19                  | 0.14     | 0.01                | 0.14       |
| (1,483)  | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 19                  | 0.14     | 0.01                | 0.14       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 19                  | 0.12     | 0.01                | 0.12       |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 18                  | 0.24     | 0.02                | 0.23       |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 18                  | 0.24     | 0.02                | 0.23       |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 18                  | 0.14     | 0.02                | 0.13       |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 18                  | 0.14     | 0.02                | 0.13       |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 18                  | 0.13     | 0.01                | 0.13       |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 18                  | 0.11     | 0.01                | 0.11       |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 17                  | 0.2      | 0.01                | 0.2        |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG22  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG23  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 17                  | 0.15     | 0.01                | 0.15       |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 17                  | 0.15     | 0.01                | 0.15       |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 17                  | 0.15     | 0.01                | 0.15       |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 16                  | 0.17     | 0.02                | 0.17       |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3   | 16                  | 0.13     | 0.02                | 0.13       |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 15                  | 0.12     | 0.02                | 0.11       |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 15                  | 0.12     | 0.02                | 0.11       |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 15                  | 0.12     | 0.02                | 0.11       |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 14                  | 0.27     | 0.06                | 0.26       |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 14                  | 0.27     | 0.06                | 0.26       |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 14                  | 0.27     | 0.06                | 0.26       |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 14                  | 0.27     | 0.06                | 0.26       |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 14                  | 0.13     | 0.02                | 0.13       |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 14                  | 0.12     | 0.01                | 0.13       |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 13                  | 0.5      | 0.01                | 0.5        |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 13                  | 0.48     | 0.01                | 0.48       |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 13                  | 0.3      | 0.01                | 0.3        |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 13                  | 0.25     | 0.02                | 0.25       |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 13                  | 0.25     | 0.02                | 0.25       |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 13                  | 0.16     | 0.01                | 0.16       |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 13                  | 0.13     | 0.01                | 0.13       |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H     | 13                  | 0.12     | 0.02                | 0.11       |
| (1,743)  | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 13                  | 0.11     | 0.01                | 0.11       |
| (1,743)  | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 13                  | 0.11     | 0.01                | 0.11       |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 12                  | 0.14     | 0.02                | 0.13       |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 12                  | 0.14     | 0.02                | 0.13       |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 12                  | 0.13     | 0.02                | 0.13       |
| (1,213)  | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 12                  | 0.12     | 0.01                | 0.12       |
| (1,67)   | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 12                  | 0.12     | 0.0                 | 0.12       |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 12                  | 0.12     | 0.02                | 0.11       |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 12                  | 0.12     | 0.02                | 0.11       |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 12                  | 0.12     | 0.02                | 0.11       |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 12                  | 0.12     | 0.02                | 0.11       |
| (1,357)  | 1:89:A:VAL:HG21 | 1:90:A:THR:HB    | 12                  | 0.11     | 0.0                 | 0.11       |
| (1,357)  | 1:89:A:VAL:HG22 | 1:90:A:THR:HB    | 12                  | 0.11     | 0.0                 | 0.11       |
| (1,357)  | 1:89:A:VAL:HG23 | 1:90:A:THR:HB    | 12                  | 0.11     | 0.0                 | 0.11       |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 11                  | 0.19     | 0.04                | 0.2        |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 11                  | 0.19     | 0.04                | 0.2        |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11  | 11                  | 0.16     | 0.02                | 0.16       |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12  | 11                  | 0.16     | 0.02                | 0.16       |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13  | 11                  | 0.16     | 0.02                | 0.16       |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11  | 11                  | 0.16     | 0.02                | 0.16       |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12  | 11                  | 0.16     | 0.02                | 0.16       |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13  | 11                  | 0.16     | 0.02                | 0.16       |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2   | 10                  | 0.35     | 0.07                | 0.36       |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2   | 10                  | 0.33     | 0.18                | 0.22       |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3   | 10                  | 0.33     | 0.18                | 0.22       |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H    | 10                  | 0.16     | 0.03                | 0.16       |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 10                  | 0.12     | 0.01                | 0.12       |
| (1,371)  | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,371)  | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,371)  | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 10                  | 0.12     | 0.01                | 0.12       |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21  | 10                  | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22  | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23  | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 9                   | 0.15     | 0.02                | 0.15       |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 9                   | 0.15     | 0.02                | 0.15       |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA    | 9                   | 0.12     | 0.02                | 0.11       |
| (1,618)  | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 8                   | 0.16     | 0.03                | 0.16       |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 8                   | 0.12     | 0.01                | 0.11       |
| (1,792)  | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,522)  | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 8                   | 0.1      | 0.0                 | 0.1        |
| (1,1666) | 1:102:A:LYS:HE2 | 1:103:A:SER:H    | 6                   | 0.17     | 0.01                | 0.16       |
| (1,1666) | 1:102:A:LYS:HE3 | 1:103:A:SER:H    | 6                   | 0.17     | 0.01                | 0.16       |
| (1,379)  | 1:28:A:ASN:H    | 1:126:A:ASN:HA   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE1   | 6                   | 0.12     | 0.01                | 0.11       |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE2   | 6                   | 0.12     | 0.01                | 0.11       |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE3   | 6                   | 0.12     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB1   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB2   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB3   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB1   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB2   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB3   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB1   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB2   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB3   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,507)  | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD11 | 6                   | 0.11     | 0.01                | 0.11       |
| (1,507)  | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD12 | 6                   | 0.11     | 0.01                | 0.11       |
| (1,507)  | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD13 | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA2   | 5                   | 0.49     | 0.1                 | 0.42       |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA3   | 5                   | 0.49     | 0.1                 | 0.42       |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA2   | 5                   | 0.49     | 0.1                 | 0.42       |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA3   | 5                   | 0.49     | 0.1                 | 0.42       |
| (1,113)  | 1:68:A:LEU:HD21 | 1:78:A:VAL:HB    | 5                   | 0.14     | 0.04                | 0.12       |
| (1,113)  | 1:68:A:LEU:HD22 | 1:78:A:VAL:HB    | 5                   | 0.14     | 0.04                | 0.12       |
| (1,113)  | 1:68:A:LEU:HD23 | 1:78:A:VAL:HB    | 5                   | 0.14     | 0.04                | 0.12       |
| (1,428)  | 1:26:A:MET:HA   | 1:127:A:LEU:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1475) | 1:31:A:GLY:H    | 1:130:A:LYS:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1641) | 1:51:A:PRO:HB2  | 1:116:A:LEU:H    | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,1185) | 1:90:A:THR:HG21 | 1:91:A:TYR:H     | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1185) | 1:90:A:THR:HG22 | 1:91:A:TYR:H     | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1185) | 1:90:A:THR:HG23 | 1:91:A:TYR:H     | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1788) | 1:9:A:TYR:H     | 1:9:A:TYR:HE2    | 4                   | 0.96     | 0.5                 | 0.96       |
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD2  | 4                   | 0.28     | 0.06                | 0.3        |

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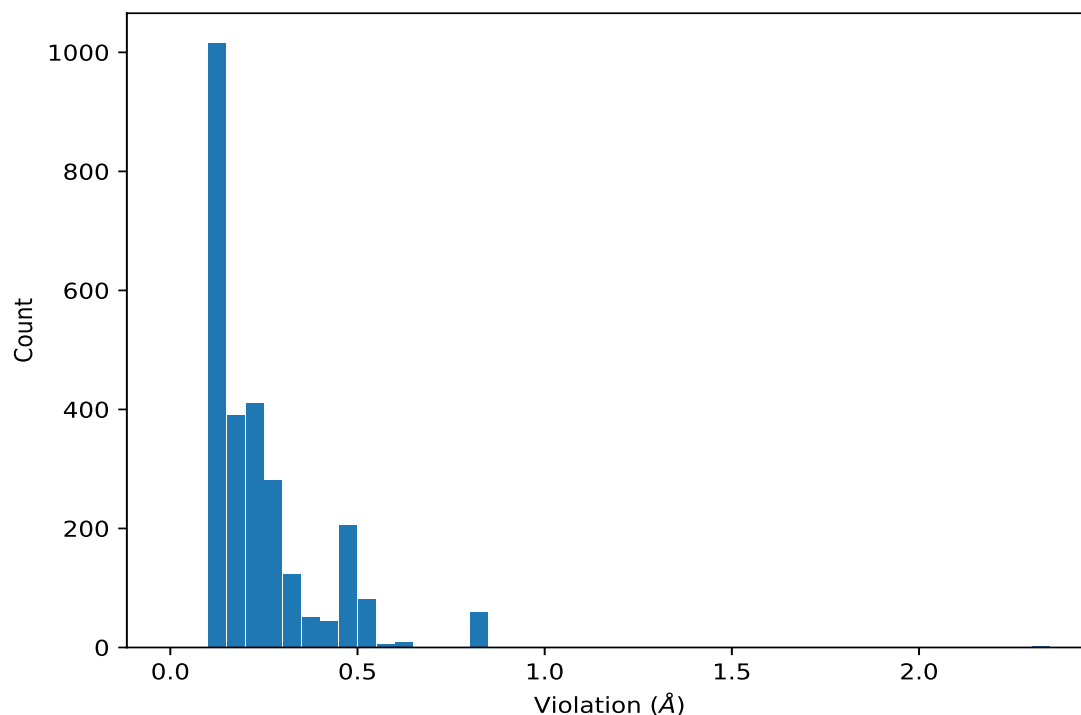
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD3 | 4                   | 0.28     | 0.06                | 0.3        |
| (1,806)  | 1:77:A:ARG:HA   | 1:136:A:LYS:HG3 | 4                   | 0.2      | 0.08                | 0.2        |
| (1,351)  | 1:67:A:ALA:HB1  | 1:71:A:THR:HB   | 4                   | 0.12     | 0.02                | 0.12       |
| (1,351)  | 1:67:A:ALA:HB2  | 1:71:A:THR:HB   | 4                   | 0.12     | 0.02                | 0.12       |
| (1,351)  | 1:67:A:ALA:HB3  | 1:71:A:THR:HB   | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1664) | 1:88:A:GLU:H    | 1:126:A:ASN:HB3 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,458)  | 1:40:A:LEU:HG   | 1:68:A:LEU:HB3  | 4                   | 0.12     | 0.01                | 0.11       |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG2 | 3                   | 0.13     | 0.03                | 0.11       |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG3 | 3                   | 0.13     | 0.03                | 0.11       |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG2 | 3                   | 0.13     | 0.03                | 0.11       |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG3 | 3                   | 0.13     | 0.03                | 0.11       |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG2 | 3                   | 0.13     | 0.03                | 0.11       |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG3 | 3                   | 0.13     | 0.03                | 0.11       |
| (1,1653) | 1:60:A:ILE:H    | 1:63:A:TYR:HB2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1657) | 1:125:A:PHE:HD1 | 1:126:A:ASN:H   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,536)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HE2  | 2                   | 0.29     | 0.0                 | 0.29       |
| (1,1633) | 1:9:A:TYR:H     | 1:11:A:LYS:H    | 2                   | 0.27     | 0.01                | 0.27       |
| (1,1856) | 1:11:A:LYS:HB2  | 1:48:A:PRO:HD2  | 2                   | 0.19     | 0.07                | 0.19       |
| (1,1856) | 1:11:A:LYS:HB2  | 1:48:A:PRO:HD3  | 2                   | 0.19     | 0.07                | 0.19       |
| (1,1856) | 1:11:A:LYS:HB3  | 1:48:A:PRO:HD2  | 2                   | 0.19     | 0.07                | 0.19       |
| (1,1856) | 1:11:A:LYS:HB3  | 1:48:A:PRO:HD3  | 2                   | 0.19     | 0.07                | 0.19       |
| (1,2148) | 1:135:A:LYS:HA  | 1:136:A:LYS:HD2 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2148) | 1:135:A:LYS:HA  | 1:136:A:LYS:HD3 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1191) | 1:78:A:VAL:HG11 | 1:80:A:GLU:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (1,1191) | 1:78:A:VAL:HG12 | 1:80:A:GLU:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (1,1191) | 1:78:A:VAL:HG13 | 1:80:A:GLU:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (1,1850) | 1:10:A:LYS:HB2  | 1:62:A:TYR:HE1  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1850) | 1:10:A:LYS:HB3  | 1:62:A:TYR:HE1  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1130) | 1:25:A:LEU:H    | 1:49:A:ILE:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,475)  | 1:102:A:LYS:HB2 | 1:104:A:PHE:HE1 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1447) | 1:79:A:VAL:H    | 1:80:A:GLU:HG2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1447) | 1:79:A:VAL:H    | 1:80:A:GLU:HG3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,423)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HE3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1777) | 1:95:A:ASN:HD21 | 1:97:A:LYS:H    | 2                   | 0.1      | 0.0                 | 0.1        |

<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) |
|----------|-----------------|----------------|----------|---------------|
| (1,1871) | 1:17:A:TYR:HE1  | 1:18:A:PHE:HB2 | 17       | 2.32          |
| (1,1871) | 1:17:A:TYR:HE1  | 1:18:A:PHE:HB3 | 17       | 2.32          |
| (1,1705) | 1:17:A:TYR:H    | 1:17:A:TYR:HE2 | 17       | 1.99          |
| (1,1788) | 1:9:A:TYR:H     | 1:9:A:TYR:HE2  | 3        | 1.47          |
| (1,1788) | 1:9:A:TYR:H     | 1:9:A:TYR:HE2  | 10       | 1.45          |
| (1,258)  | 1:45:A:VAL:HG21 | 1:46:A:GLU:H   | 8        | 0.82          |
| (1,258)  | 1:45:A:VAL:HG22 | 1:46:A:GLU:H   | 8        | 0.82          |
| (1,258)  | 1:45:A:VAL:HG23 | 1:46:A:GLU:H   | 8        | 0.82          |
| (1,258)  | 1:45:A:VAL:HG21 | 1:46:A:GLU:H   | 10       | 0.82          |
| (1,258)  | 1:45:A:VAL:HG22 | 1:46:A:GLU:H   | 10       | 0.82          |

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| Key     | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|---------|-----------------|--------------|----------|---------------|
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 10       | 0.82          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 14       | 0.82          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 14       | 0.82          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 14       | 0.82          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 16       | 0.82          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 16       | 0.82          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 16       | 0.82          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 1        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 1        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 1        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 2        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 2        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 2        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 3        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 3        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 3        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 4        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 4        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 4        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 5        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 5        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 5        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 6        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 6        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 6        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 7        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 7        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 7        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 9        | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 9        | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 9        | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 11       | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 11       | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 11       | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 12       | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 12       | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 12       | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 13       | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 13       | 0.81          |
| (1,258) | 1:45:A:VAL:HG23 | 1:46:A:GLU:H | 13       | 0.81          |
| (1,258) | 1:45:A:VAL:HG21 | 1:46:A:GLU:H | 15       | 0.81          |
| (1,258) | 1:45:A:VAL:HG22 | 1:46:A:GLU:H | 15       | 0.81          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,258)  | 1:45:A:VAL:HG23 | 1:46:A:GLU:H    | 15       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG21 | 1:46:A:GLU:H    | 17       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG22 | 1:46:A:GLU:H    | 17       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG23 | 1:46:A:GLU:H    | 17       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG21 | 1:46:A:GLU:H    | 18       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG22 | 1:46:A:GLU:H    | 18       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG23 | 1:46:A:GLU:H    | 18       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG21 | 1:46:A:GLU:H    | 19       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG22 | 1:46:A:GLU:H    | 19       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG23 | 1:46:A:GLU:H    | 19       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG21 | 1:46:A:GLU:H    | 20       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG22 | 1:46:A:GLU:H    | 20       | 0.81          |
| (1,258)  | 1:45:A:VAL:HG23 | 1:46:A:GLU:H    | 20       | 0.81          |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA2  | 10       | 0.62          |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA3  | 10       | 0.62          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA2  | 10       | 0.62          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA3  | 10       | 0.62          |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA2  | 14       | 0.61          |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA3  | 14       | 0.61          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA2  | 14       | 0.61          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA3  | 14       | 0.61          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2  | 14       | 0.61          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3  | 14       | 0.61          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2  | 10       | 0.6           |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3  | 10       | 0.6           |
| (1,1177) | 1:61:A:GLU:HB3  | 1:62:A:TYR:H    | 9        | 0.59          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2  | 4        | 0.58          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3  | 4        | 0.58          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11 | 9        | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12 | 9        | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13 | 9        | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11 | 12       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12 | 12       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13 | 12       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11 | 13       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12 | 13       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13 | 13       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11 | 16       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12 | 16       | 0.52          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13 | 16       | 0.52          |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H   | 2        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11 | 1        | 0.51          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 1        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 1        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 2        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 2        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 2        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 3        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 3        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 3        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 4        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 4        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 4        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 5        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 5        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 5        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 6        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 6        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 6        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 7        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 7        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 7        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 8        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 8        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 8        | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 11       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 11       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 11       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 15       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 15       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 15       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 17       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 17       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 17       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 18       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 18       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 18       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 19       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 19       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 19       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 20       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 20       | 0.51          |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 20       | 0.51          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 15       | 0.5           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 15       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 15       | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 1        | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 3        | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 7        | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 8        | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 9        | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 12       | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 19       | 0.5           |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 20       | 0.5           |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 10       | 0.5           |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 10       | 0.5           |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 10       | 0.5           |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG11  | 14       | 0.5           |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG12  | 14       | 0.5           |
| (1,461)  | 1:44:A:TYR:HA   | 1:45:A:VAL:HG13  | 14       | 0.5           |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 6        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 7        | 0.49          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 7        | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 12       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 12       | 0.49          |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 4        | 0.49          |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 6        | 0.49          |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 13       | 0.49          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 2        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 4        | 0.48          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 4        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 8        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 9        | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 13       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 19       | 0.48          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 19       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 19       | 0.48          |
| (1,1167) | 1:102:A:LYS:HB2 | 1:103:A:SER:H    | 15       | 0.48          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 1        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 3        | 0.47          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 3        | 0.47          |
| (1,1788) | 1:9:A:TYR:H     | 1:9:A:TYR:HE2    | 17       | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 2        | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 2        | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 2        | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 10       | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 10       | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 10       | 0.47          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 13       | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 13       | 0.47          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 13       | 0.47          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD11 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD12 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD13 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD21 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD22 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE2 | 1:116:A:LEU:HD23 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD11 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD12 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD13 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD21 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD22 | 20       | 0.46          |
| (1,2076) | 1:102:A:LYS:HE3 | 1:116:A:LEU:HD23 | 20       | 0.46          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 9        | 0.46          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 9        | 0.46          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 9        | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 7        | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 7        | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 7        | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 9        | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 9        | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 9        | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 14       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 14       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 14       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 19       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 19       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 19       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 20       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 20       | 0.46          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 20       | 0.46          |
| (1,1788) | 1:9:A:TYR:H     | 1:9:A:TYR:HE2    | 5        | 0.45          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 12       | 0.45          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 12       | 0.45          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 12       | 0.45          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2   | 13       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 3        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG22  | 3        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG23  | 3        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB   | 1:45:A:VAL:HG21  | 4        | 0.45          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 4        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 4        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 5        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 5        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 5        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 6        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 6        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 6        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 8        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 8        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 8        | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 12       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 12       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 12       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 16       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 16       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 16       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 17       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 17       | 0.45          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 17       | 0.45          |
| (1,1219) | 1:26:A:MET:HE1 | 1:127:A:LEU:H   | 1        | 0.44          |
| (1,1219) | 1:26:A:MET:HE2 | 1:127:A:LEU:H   | 1        | 0.44          |
| (1,1219) | 1:26:A:MET:HE3 | 1:127:A:LEU:H   | 1        | 0.44          |
| (1,1219) | 1:26:A:MET:HE1 | 1:127:A:LEU:H   | 6        | 0.44          |
| (1,1219) | 1:26:A:MET:HE2 | 1:127:A:LEU:H   | 6        | 0.44          |
| (1,1219) | 1:26:A:MET:HE3 | 1:127:A:LEU:H   | 6        | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 1        | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 1        | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 1        | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 11       | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 11       | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 11       | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 15       | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 15       | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 15       | 0.44          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG21 | 18       | 0.43          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG22 | 18       | 0.43          |
| (1,334)  | 1:27:A:VAL:HB  | 1:45:A:VAL:HG23 | 18       | 0.43          |
| (1,1859) | 1:11:A:LYS:HD2 | 1:12:A:GLY:HA2  | 3        | 0.42          |
| (1,1859) | 1:11:A:LYS:HD2 | 1:12:A:GLY:HA3  | 3        | 0.42          |
| (1,1859) | 1:11:A:LYS:HD3 | 1:12:A:GLY:HA2  | 3        | 0.42          |
| (1,1859) | 1:11:A:LYS:HD3 | 1:12:A:GLY:HA3  | 3        | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H   | 5        | 0.42          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H   | 5        | 0.42          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H   | 5        | 0.42          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H   | 11       | 0.42          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H   | 11       | 0.42          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H   | 11       | 0.42          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H   | 14       | 0.42          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H   | 14       | 0.42          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H   | 14       | 0.42          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H   | 17       | 0.42          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H   | 17       | 0.42          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H   | 17       | 0.42          |
| (1,2090) | 1:109:A:LYS:H   | 1:109:A:LYS:HE2 | 19       | 0.41          |
| (1,2090) | 1:109:A:LYS:H   | 1:109:A:LYS:HE3 | 19       | 0.41          |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA2  | 16       | 0.41          |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA3  | 16       | 0.41          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA2  | 16       | 0.41          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA3  | 16       | 0.41          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2  | 15       | 0.4           |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3  | 15       | 0.4           |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2  | 15       | 0.4           |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3  | 15       | 0.4           |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 3        | 0.4           |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA2  | 2        | 0.39          |
| (1,1859) | 1:11:A:LYS:HD2  | 1:12:A:GLY:HA3  | 2        | 0.39          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA2  | 2        | 0.39          |
| (1,1859) | 1:11:A:LYS:HD3  | 1:12:A:GLY:HA3  | 2        | 0.39          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 5        | 0.39          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 1        | 0.39          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 7        | 0.39          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2  | 20       | 0.39          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2  | 17       | 0.38          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3  | 17       | 0.38          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2  | 17       | 0.38          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3  | 17       | 0.38          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 6        | 0.38          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 4        | 0.38          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 8        | 0.38          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 1        | 0.37          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 3        | 0.37          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 12       | 0.37          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 19       | 0.37          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 2        | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 6        | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 10       | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 11       | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 13       | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 14       | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 17       | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 19       | 0.37          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 20       | 0.37          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2 | 9        | 0.37          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2 | 12       | 0.37          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA | 5        | 0.36          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA | 5        | 0.36          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA | 18       | 0.36          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA | 18       | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 2        | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 4        | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 8        | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 10       | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 11       | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 13       | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 14       | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 15       | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 16       | 0.36          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H   | 17       | 0.36          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2 | 19       | 0.36          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3 | 19       | 0.36          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 12       | 0.36          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 15       | 0.36          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H   | 18       | 0.36          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2 | 11       | 0.36          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2 | 15       | 0.36          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA | 9        | 0.35          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA | 9        | 0.35          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA | 13       | 0.35          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA | 13       | 0.35          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA | 15       | 0.35          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA | 15       | 0.35          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA | 16       | 0.35          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA | 16       | 0.35          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2 | 4        | 0.35          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3 | 4        | 0.35          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2  | 4        | 0.35          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3  | 4        | 0.35          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2 | 15       | 0.35          |
| (1,1618) | 1:31:A:GLY:H    | 1:131:A:VAL:HB  | 7        | 0.35          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 7        | 0.35          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 9        | 0.35          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 18       | 0.35          |
| (1,1477) | 1:87:A:ILE:HG12 | 1:88:A:GLU:H    | 20       | 0.35          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 9        | 0.35          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 16       | 0.35          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2  | 6        | 0.35          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA  | 11       | 0.34          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA  | 11       | 0.34          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA  | 20       | 0.34          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA  | 20       | 0.34          |
| (1,1197) | 1:77:A:ARG:HB2  | 1:78:A:VAL:H    | 5        | 0.34          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2  | 18       | 0.34          |
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD2 | 6        | 0.33          |
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD3 | 6        | 0.33          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA  | 12       | 0.33          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA  | 12       | 0.33          |
| (1,1978) | 1:61:A:GLU:HB2  | 1:62:A:TYR:H    | 9        | 0.33          |
| (1,1978) | 1:61:A:GLU:HB3  | 1:62:A:TYR:H    | 9        | 0.33          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13 | 15       | 0.33          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13 | 15       | 0.33          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13 | 15       | 0.33          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13 | 15       | 0.33          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13 | 15       | 0.33          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13 | 15       | 0.33          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2  | 16       | 0.33          |
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD2 | 1        | 0.32          |
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD3 | 1        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 1        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 1        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 2        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 2        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 3        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 3        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 4        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 4        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 6        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 6        | 0.32          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 7        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 7        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 9        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 9        | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 12       | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 12       | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 13       | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 13       | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 15       | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 15       | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 19       | 0.32          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 19       | 0.32          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 7        | 0.32          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 8        | 0.32          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 9        | 0.32          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 6        | 0.32          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 6        | 0.32          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 6        | 0.32          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 11       | 0.32          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 11       | 0.32          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 11       | 0.32          |
| (1,806)  | 1:77:A:ARG:HA   | 1:136:A:LYS:HG3  | 6        | 0.32          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 7        | 0.32          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 8        | 0.32          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 6        | 0.31          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 6        | 0.31          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 8        | 0.31          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 8        | 0.31          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 20       | 0.31          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 20       | 0.31          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 5        | 0.31          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 5        | 0.31          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 8        | 0.31          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 8        | 0.31          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 10       | 0.31          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 10       | 0.31          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 9        | 0.31          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 9        | 0.31          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 9        | 0.31          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 9        | 0.31          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 9        | 0.31          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 9        | 0.31          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 20       | 0.31          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 20       | 0.31          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 20       | 0.31          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 20       | 0.31          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 20       | 0.31          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 20       | 0.31          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 16       | 0.31          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 3        | 0.31          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 19       | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 2        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 2        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 2        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 3        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 3        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 3        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 5        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 5        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 5        | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 12       | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 12       | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 12       | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 19       | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 19       | 0.31          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 19       | 0.31          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 12       | 0.31          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 12       | 0.31          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 12       | 0.31          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 15       | 0.31          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 20       | 0.31          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 6        | 0.3           |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 6        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 3        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 3        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 3        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 3        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 3        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 3        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 8        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 8        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 8        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 8        | 0.3           |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 8        | 0.3           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 8        | 0.3           |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 19       | 0.3           |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 19       | 0.3           |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 19       | 0.3           |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 19       | 0.3           |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 4        | 0.3           |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 7        | 0.3           |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 11       | 0.3           |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 1        | 0.3           |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 2        | 0.3           |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 12       | 0.3           |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 13       | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 1        | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 1        | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 1        | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 4        | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 4        | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 4        | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 14       | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 14       | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 14       | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 20       | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 20       | 0.3           |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 20       | 0.3           |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 16       | 0.3           |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 16       | 0.3           |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 16       | 0.3           |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 4        | 0.3           |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 9        | 0.3           |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 13       | 0.3           |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 19       | 0.29          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 19       | 0.29          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 1        | 0.29          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 1        | 0.29          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 1        | 0.29          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 1        | 0.29          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 1        | 0.29          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 1        | 0.29          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 14       | 0.29          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 8        | 0.29          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 9        | 0.29          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 10       | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 20       | 0.29          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 16       | 0.29          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 13       | 0.29          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 13       | 0.29          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 13       | 0.29          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 16       | 0.29          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 16       | 0.29          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 16       | 0.29          |
| (1,536)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HE2   | 20       | 0.29          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 1        | 0.29          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 2        | 0.29          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 6        | 0.29          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 19       | 0.29          |
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD2  | 3        | 0.28          |
| (1,2157) | 1:136:A:LYS:HA  | 1:136:A:LYS:HD3  | 3        | 0.28          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 6        | 0.28          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 6        | 0.28          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 2        | 0.28          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 2        | 0.28          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 4        | 0.28          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 4        | 0.28          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 17       | 0.28          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 17       | 0.28          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 7        | 0.28          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 7        | 0.28          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 7        | 0.28          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 7        | 0.28          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 7        | 0.28          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 7        | 0.28          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 18       | 0.28          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 18       | 0.28          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 18       | 0.28          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 18       | 0.28          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 18       | 0.28          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 18       | 0.28          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 7        | 0.28          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 7        | 0.28          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 7        | 0.28          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 7        | 0.28          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 8        | 0.28          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 8        | 0.28          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 8        | 0.28          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 8        | 0.28          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 4        | 0.28          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 18       | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 1        | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 2        | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 3        | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 11       | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 13       | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 15       | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 17       | 0.28          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 19       | 0.28          |
| (1,1633) | 1:9:A:TYR:H     | 1:11:A:LYS:H     | 10       | 0.28          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 4        | 0.28          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 6        | 0.28          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 10       | 0.28          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 18       | 0.28          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 20       | 0.28          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 4        | 0.28          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 6        | 0.28          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 17       | 0.28          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 20       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 7        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 7        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 7        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 8        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 8        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 8        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 9        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 9        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 9        | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 15       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 15       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 15       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 17       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 17       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 17       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 18       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 18       | 0.28          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 18       | 0.28          |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 11       | 0.28          |
| (1,536)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HE2   | 11       | 0.28          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 12       | 0.28          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 12       | 0.27          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 12       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 10       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 10       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 11       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 11       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 14       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 14       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 16       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 16       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 17       | 0.27          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 17       | 0.27          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 7        | 0.27          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 7        | 0.27          |
| (1,1997) | 1:77:A:ARG:HD2  | 1:136:A:LYS:HA   | 14       | 0.27          |
| (1,1997) | 1:77:A:ARG:HD3  | 1:136:A:LYS:HA   | 14       | 0.27          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 6        | 0.27          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 6        | 0.27          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 6        | 0.27          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 6        | 0.27          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 6        | 0.27          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 6        | 0.27          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 12       | 0.27          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 12       | 0.27          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 12       | 0.27          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 12       | 0.27          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 12       | 0.27          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 12       | 0.27          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 16       | 0.27          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 18       | 0.27          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 5        | 0.27          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 6        | 0.27          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 12       | 0.27          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 14       | 0.27          |
| (1,1668) | 1:27:A:VAL:H    | 1:127:A:LEU:H    | 18       | 0.27          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 9        | 0.27          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 7        | 0.27          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 15       | 0.27          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 5        | 0.27          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 16       | 0.27          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG11 | 10       | 0.27          |
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG12 | 10       | 0.27          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1113) | 1:53:A:THR:H    | 1:112:A:VAL:HG13 | 10       | 0.27          |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 20       | 0.27          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 20       | 0.27          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 20       | 0.27          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 20       | 0.27          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 9        | 0.27          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 9        | 0.27          |
| (1,384)  | 1:102:A:LYS:HG2 | 1:104:A:PHE:HZ   | 3        | 0.27          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 1        | 0.26          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 1        | 0.26          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 4        | 0.26          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 4        | 0.26          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 13       | 0.26          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 13       | 0.26          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 18       | 0.26          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 18       | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 4        | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 4        | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 4        | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 4        | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 4        | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 4        | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 14       | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 14       | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 14       | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 14       | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 14       | 0.26          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 14       | 0.26          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 19       | 0.26          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 19       | 0.26          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 19       | 0.26          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 19       | 0.26          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 19       | 0.26          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 19       | 0.26          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 1        | 0.26          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 1        | 0.26          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 1        | 0.26          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 1        | 0.26          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 5        | 0.26          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 5        | 0.26          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 5        | 0.26          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 5        | 0.26          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1856) | 1:11:A:LYS:HB2  | 1:48:A:PRO:HD2   | 15       | 0.26          |
| (1,1856) | 1:11:A:LYS:HB2  | 1:48:A:PRO:HD3   | 15       | 0.26          |
| (1,1856) | 1:11:A:LYS:HB3  | 1:48:A:PRO:HD2   | 15       | 0.26          |
| (1,1856) | 1:11:A:LYS:HB3  | 1:48:A:PRO:HD3   | 15       | 0.26          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 5        | 0.26          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 11       | 0.26          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 15       | 0.26          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 16       | 0.26          |
| (1,1633) | 1:9:A:TYR:H     | 1:11:A:LYS:H     | 3        | 0.26          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 20       | 0.26          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 3        | 0.26          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 5        | 0.26          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 14       | 0.26          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 17       | 0.26          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 9        | 0.26          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 9        | 0.26          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 9        | 0.26          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 3        | 0.25          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 3        | 0.25          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 11       | 0.25          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 11       | 0.25          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 2        | 0.25          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 2        | 0.25          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 15       | 0.25          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 15       | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 1        | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 1        | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 1        | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 1        | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 1        | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 1        | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 12       | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 12       | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 12       | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 12       | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 12       | 0.25          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 12       | 0.25          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 18       | 0.25          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 18       | 0.25          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 18       | 0.25          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 18       | 0.25          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 1        | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 10       | 0.25          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 13       | 0.25          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 6        | 0.25          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 9        | 0.25          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 11       | 0.25          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 12       | 0.25          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 20       | 0.25          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 1        | 0.25          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 6        | 0.25          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 7        | 0.25          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 12       | 0.25          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 1        | 0.25          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 8        | 0.25          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 9        | 0.25          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 12       | 0.25          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2   | 13       | 0.25          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 5        | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 5        | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 9        | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 9        | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 16       | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 16       | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 20       | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 20       | 0.24          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2  | 10       | 0.24          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3  | 10       | 0.24          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 8        | 0.24          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 8        | 0.24          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD2  | 19       | 0.24          |
| (1,2073) | 1:102:A:LYS:H   | 1:102:A:LYS:HD3  | 19       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 2        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 2        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 2        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 2        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 2        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 2        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 3        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 3        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 3        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 3        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 3        | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 3        | 0.24          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 11       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 11       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 11       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 11       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 11       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 11       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 16       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 16       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 16       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 16       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 16       | 0.24          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 16       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 2        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 2        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 2        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 2        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 2        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 2        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 4        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 4        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 4        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 4        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 4        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 4        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 5        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 5        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 5        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 5        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 5        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 5        | 0.24          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 11       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 11       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 11       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 11       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 11       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 11       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 14       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 14       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 14       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 14       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 14       | 0.24          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 14       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2  | 11       | 0.24          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3  | 11       | 0.24          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2  | 11       | 0.24          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3  | 11       | 0.24          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2 | 6        | 0.24          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2 | 7        | 0.24          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2 | 9        | 0.24          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H   | 4        | 0.24          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H   | 13       | 0.24          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2  | 2        | 0.24          |
| (1,1464) | 1:95:A:ASN:HD22 | 1:96:A:LYS:HG2  | 19       | 0.24          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2  | 10       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 6        | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 6        | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 6        | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 10       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 10       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 10       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 11       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 11       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 11       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 15       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 15       | 0.24          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 15       | 0.24          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2 | 4        | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3 | 4        | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2 | 8        | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3 | 8        | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2 | 12       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3 | 12       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2 | 14       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3 | 14       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2 | 15       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3 | 15       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2 | 17       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3 | 17       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2 | 19       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3 | 19       | 0.23          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 11       | 0.23          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 11       | 0.23          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 14       | 0.23          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 14       | 0.23          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2077) | 1:103:A:SER:H  | 1:103:A:SER:HB2  | 17       | 0.23          |
| (1,2077) | 1:103:A:SER:H  | 1:103:A:SER:HB3  | 17       | 0.23          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD2  | 3        | 0.23          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD3  | 3        | 0.23          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD2  | 7        | 0.23          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD3  | 7        | 0.23          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD2  | 9        | 0.23          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD3  | 9        | 0.23          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD2   | 3        | 0.23          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD3   | 3        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 7        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 7        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 7        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 7        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 7        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 7        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 8        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 8        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 8        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 8        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 8        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 8        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 9        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 9        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 9        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 9        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 9        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 9        | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 10       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 10       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 10       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 10       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 10       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 10       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 15       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 15       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 15       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 15       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 15       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 15       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 19       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 19       | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 19       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 19       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 19       | 0.23          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 19       | 0.23          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 17       | 0.23          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 17       | 0.23          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 17       | 0.23          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 17       | 0.23          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 17       | 0.23          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 17       | 0.23          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 6        | 0.23          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 6        | 0.23          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 6        | 0.23          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 6        | 0.23          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 9        | 0.23          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 9        | 0.23          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 9        | 0.23          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 9        | 0.23          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 19       | 0.23          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 20       | 0.23          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 5        | 0.23          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 8        | 0.23          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 15       | 0.23          |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 20       | 0.23          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 3        | 0.23          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 3        | 0.23          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 3        | 0.23          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 13       | 0.23          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 13       | 0.23          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 13       | 0.23          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 18       | 0.23          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 18       | 0.23          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 18       | 0.23          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 10       | 0.23          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 13       | 0.23          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 13       | 0.23          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 2        | 0.22          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 2        | 0.22          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 7        | 0.22          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 7        | 0.22          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE2  | 10       | 0.22          |
| (1,2156) | 1:136:A:LYS:H   | 1:136:A:LYS:HE3  | 10       | 0.22          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2156) | 1:136:A:LYS:H  | 1:136:A:LYS:HE2  | 18       | 0.22          |
| (1,2156) | 1:136:A:LYS:H  | 1:136:A:LYS:HE3  | 18       | 0.22          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD2  | 20       | 0.22          |
| (1,2073) | 1:102:A:LYS:H  | 1:102:A:LYS:HD3  | 20       | 0.22          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD2   | 2        | 0.22          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD3   | 2        | 0.22          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD2   | 7        | 0.22          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD3   | 7        | 0.22          |
| (1,1997) | 1:77:A:ARG:HD2 | 1:136:A:LYS:HA   | 1        | 0.22          |
| (1,1997) | 1:77:A:ARG:HD3 | 1:136:A:LYS:HA   | 1        | 0.22          |
| (1,1997) | 1:77:A:ARG:HD2 | 1:136:A:LYS:HA   | 3        | 0.22          |
| (1,1997) | 1:77:A:ARG:HD3 | 1:136:A:LYS:HA   | 3        | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 5        | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 5        | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 5        | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 5        | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 5        | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 5        | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 13       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 13       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 13       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 13       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 13       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 13       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 17       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 17       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 17       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 17       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 17       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 17       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 18       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 18       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 18       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 18       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 18       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 18       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG11 | 20       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG12 | 20       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG13 | 20       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG21 | 20       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG22 | 20       | 0.22          |
| (1,1928) | 1:31:A:GLY:HA3 | 1:131:A:VAL:HG23 | 20       | 0.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 13       | 0.22          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 13       | 0.22          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 13       | 0.22          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 13       | 0.22          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 13       | 0.22          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 13       | 0.22          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 13       | 0.22          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 13       | 0.22          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 13       | 0.22          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 13       | 0.22          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 2        | 0.22          |
| (1,1804) | 1:121:A:LYS:H   | 1:122:A:ASN:HB2  | 17       | 0.22          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 3        | 0.22          |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 11       | 0.22          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2   | 7        | 0.22          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3   | 7        | 0.22          |
| (1,806)  | 1:77:A:ARG:HA   | 1:136:A:LYS:HG3  | 3        | 0.22          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 11       | 0.22          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 11       | 0.22          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 18       | 0.22          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 18       | 0.22          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 16       | 0.22          |
| (1,2084) | 1:108:A:GLU:H   | 1:109:A:LYS:HE2  | 19       | 0.21          |
| (1,2084) | 1:108:A:GLU:H   | 1:109:A:LYS:HE3  | 19       | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 6        | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 6        | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 8        | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 8        | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 12       | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 12       | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 13       | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 13       | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2   | 19       | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3   | 19       | 0.21          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG11 | 6        | 0.21          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG12 | 6        | 0.21          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG13 | 6        | 0.21          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG21 | 6        | 0.21          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG22 | 6        | 0.21          |
| (1,1928) | 1:31:A:GLY:HA3  | 1:131:A:VAL:HG23 | 6        | 0.21          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11  | 5        | 0.21          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12  | 5        | 0.21          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 5        | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 5        | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 5        | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 5        | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11  | 11       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12  | 11       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 11       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 11       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 11       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 11       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11  | 16       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12  | 16       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 16       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 16       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 16       | 0.21          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 16       | 0.21          |
| (1,1804) | 1:121:A:LYS:H  | 1:122:A:ASN:HB2  | 3        | 0.21          |
| (1,1804) | 1:121:A:LYS:H  | 1:122:A:ASN:HB2  | 12       | 0.21          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 9        | 0.21          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 9        | 0.21          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 9        | 0.21          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 20       | 0.21          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 20       | 0.21          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 20       | 0.21          |
| (1,1481) | 1:87:A:ILE:HA  | 1:126:A:ASN:H    | 2        | 0.21          |
| (1,1481) | 1:87:A:ILE:HA  | 1:126:A:ASN:H    | 19       | 0.21          |
| (1,1383) | 1:94:A:LYS:H   | 1:97:A:LYS:HG3   | 1        | 0.21          |
| (1,1383) | 1:94:A:LYS:H   | 1:97:A:LYS:HG3   | 3        | 0.21          |
| (1,1383) | 1:94:A:LYS:H   | 1:97:A:LYS:HG3   | 7        | 0.21          |
| (1,1383) | 1:94:A:LYS:H   | 1:97:A:LYS:HG3   | 12       | 0.21          |
| (1,1353) | 1:74:A:LYS:H   | 1:74:A:LYS:HB2   | 2        | 0.21          |
| (1,1353) | 1:74:A:LYS:H   | 1:74:A:LYS:HB3   | 2        | 0.21          |
| (1,1353) | 1:74:A:LYS:H   | 1:74:A:LYS:HB2   | 3        | 0.21          |
| (1,1353) | 1:74:A:LYS:H   | 1:74:A:LYS:HB3   | 3        | 0.21          |
| (1,1353) | 1:74:A:LYS:H   | 1:74:A:LYS:HB2   | 17       | 0.21          |
| (1,1353) | 1:74:A:LYS:H   | 1:74:A:LYS:HB3   | 17       | 0.21          |
| (1,1219) | 1:26:A:MET:HE1 | 1:127:A:LEU:H    | 15       | 0.21          |
| (1,1219) | 1:26:A:MET:HE2 | 1:127:A:LEU:H    | 15       | 0.21          |
| (1,1219) | 1:26:A:MET:HE3 | 1:127:A:LEU:H    | 15       | 0.21          |
| (1,1219) | 1:26:A:MET:HE1 | 1:127:A:LEU:H    | 18       | 0.21          |
| (1,1219) | 1:26:A:MET:HE2 | 1:127:A:LEU:H    | 18       | 0.21          |
| (1,1219) | 1:26:A:MET:HE3 | 1:127:A:LEU:H    | 18       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3 | 2        | 0.21          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3 | 3        | 0.21          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3 | 9        | 0.21          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3 | 13       | 0.21          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3 | 19       | 0.21          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3 | 20       | 0.21          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 7        | 0.21          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 13       | 0.21          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 16       | 0.21          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 19       | 0.21          |
| (1,113)  | 1:68:A:LEU:HD21 | 1:78:A:VAL:HB   | 7        | 0.21          |
| (1,113)  | 1:68:A:LEU:HD22 | 1:78:A:VAL:HB   | 7        | 0.21          |
| (1,113)  | 1:68:A:LEU:HD23 | 1:78:A:VAL:HB   | 7        | 0.21          |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2  | 1        | 0.2           |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3  | 1        | 0.2           |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2  | 4        | 0.2           |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3  | 4        | 0.2           |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2  | 15       | 0.2           |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3  | 15       | 0.2           |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD2  | 20       | 0.2           |
| (1,2021) | 1:86:A:LYS:H    | 1:86:A:LYS:HD3  | 20       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11 | 10       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12 | 10       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13 | 10       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21 | 10       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG22 | 10       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG23 | 10       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11 | 14       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12 | 14       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13 | 14       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21 | 14       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG22 | 14       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG23 | 14       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11 | 17       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12 | 17       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13 | 17       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21 | 17       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG22 | 17       | 0.2           |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG23 | 17       | 0.2           |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13 | 16       | 0.2           |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13 | 16       | 0.2           |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13 | 16       | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 16       | 0.2           |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 16       | 0.2           |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 16       | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 2        | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 2        | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 2        | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 6        | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 6        | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 6        | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 15       | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 15       | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 15       | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 16       | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 16       | 0.2           |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 16       | 0.2           |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 3        | 0.2           |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 2        | 0.2           |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 4        | 0.2           |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 6        | 0.2           |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 8        | 0.2           |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 9        | 0.2           |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 13       | 0.2           |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 19       | 0.2           |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 4        | 0.2           |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 7        | 0.2           |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 8        | 0.2           |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 12       | 0.2           |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 14       | 0.2           |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 15       | 0.2           |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 1        | 0.2           |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 6        | 0.2           |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 10       | 0.2           |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 12       | 0.2           |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 16       | 0.2           |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 2        | 0.2           |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 4        | 0.2           |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 8        | 0.2           |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 20       | 0.2           |
| (1,618)  | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 10       | 0.2           |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H    | 9        | 0.2           |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 6        | 0.2           |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 6        | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,511)  | 1:11:A:LYS:HA  | 1:48:A:PRO:HG2  | 17       | 0.2           |
| (1,511)  | 1:11:A:LYS:HA  | 1:48:A:PRO:HG3  | 17       | 0.2           |
| (1,266)  | 1:28:A:ASN:HB3 | 1:126:A:ASN:HB2 | 10       | 0.2           |
| (1,266)  | 1:28:A:ASN:HB3 | 1:126:A:ASN:HB2 | 18       | 0.2           |
| (1,254)  | 1:4:A:PHE:HA   | 1:4:A:PHE:HD1   | 11       | 0.2           |
| (1,254)  | 1:4:A:PHE:HA   | 1:4:A:PHE:HD2   | 11       | 0.2           |
| (1,2157) | 1:136:A:LYS:HA | 1:136:A:LYS:HD2 | 13       | 0.19          |
| (1,2157) | 1:136:A:LYS:HA | 1:136:A:LYS:HD3 | 13       | 0.19          |
| (1,2148) | 1:135:A:LYS:HA | 1:136:A:LYS:HD2 | 1        | 0.19          |
| (1,2148) | 1:135:A:LYS:HA | 1:136:A:LYS:HD3 | 1        | 0.19          |
| (1,2077) | 1:103:A:SER:H  | 1:103:A:SER:HB2 | 16       | 0.19          |
| (1,2077) | 1:103:A:SER:H  | 1:103:A:SER:HB3 | 16       | 0.19          |
| (1,2075) | 1:102:A:LYS:HA | 1:103:A:SER:HB2 | 10       | 0.19          |
| (1,2075) | 1:102:A:LYS:HA | 1:103:A:SER:HB3 | 10       | 0.19          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD2  | 9        | 0.19          |
| (1,2021) | 1:86:A:LYS:H   | 1:86:A:LYS:HD3  | 9        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD2 | 1:79:A:VAL:HG11 | 5        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD2 | 1:79:A:VAL:HG12 | 5        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD2 | 1:79:A:VAL:HG13 | 5        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD3 | 1:79:A:VAL:HG11 | 5        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD3 | 1:79:A:VAL:HG12 | 5        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD3 | 1:79:A:VAL:HG13 | 5        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD2 | 1:79:A:VAL:HG11 | 6        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD2 | 1:79:A:VAL:HG12 | 6        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD2 | 1:79:A:VAL:HG13 | 6        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD3 | 1:79:A:VAL:HG11 | 6        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD3 | 1:79:A:VAL:HG12 | 6        | 0.19          |
| (1,1996) | 1:77:A:ARG:HD3 | 1:79:A:VAL:HG13 | 6        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11 | 1        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12 | 1        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13 | 1        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21 | 1        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22 | 1        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23 | 1        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11 | 8        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12 | 8        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13 | 8        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21 | 8        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22 | 8        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23 | 8        | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11 | 12       | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12 | 12       | 0.19          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 12       | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 12       | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 12       | 0.19          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 12       | 0.19          |
| (1,1804) | 1:121:A:LYS:H  | 1:122:A:ASN:HB2  | 8        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 1        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 1        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 1        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 3        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 3        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 3        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 7        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 7        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 7        | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 10       | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 10       | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 10       | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 12       | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 12       | 0.19          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 12       | 0.19          |
| (1,1481) | 1:87:A:ILE:HA  | 1:126:A:ASN:H    | 11       | 0.19          |
| (1,1481) | 1:87:A:ILE:HA  | 1:126:A:ASN:H    | 17       | 0.19          |
| (1,1383) | 1:94:A:LYS:H   | 1:97:A:LYS:HG3   | 5        | 0.19          |
| (1,1383) | 1:94:A:LYS:H   | 1:97:A:LYS:HG3   | 17       | 0.19          |
| (1,1303) | 1:96:A:LYS:H   | 1:96:A:LYS:HG2   | 11       | 0.19          |
| (1,1173) | 1:26:A:MET:HB2 | 1:27:A:VAL:H     | 5        | 0.19          |
| (1,1173) | 1:26:A:MET:HB2 | 1:27:A:VAL:H     | 11       | 0.19          |
| (1,1173) | 1:26:A:MET:HB2 | 1:27:A:VAL:H     | 12       | 0.19          |
| (1,1033) | 1:118:A:GLU:H  | 1:118:A:GLU:HB3  | 1        | 0.19          |
| (1,1033) | 1:118:A:GLU:H  | 1:118:A:GLU:HB3  | 6        | 0.19          |
| (1,1033) | 1:118:A:GLU:H  | 1:118:A:GLU:HB3  | 17       | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 3        | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 4        | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 5        | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 7        | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 8        | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 9        | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 13       | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 15       | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 17       | 0.19          |
| (1,898)  | 1:97:A:LYS:H   | 1:97:A:LYS:HG3   | 19       | 0.19          |
| (1,787)  | 1:40:A:LEU:HA  | 1:76:A:PHE:HE1   | 13       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2  | 13       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 5        | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 5        | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 5        | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 7        | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 7        | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 7        | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 14       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 14       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 14       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 17       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 17       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 17       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21 | 19       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 19       | 0.19          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 19       | 0.19          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 15       | 0.19          |
| (1,618)  | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3  | 16       | 0.19          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H   | 5        | 0.19          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H   | 6        | 0.19          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2 | 3        | 0.19          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2 | 8        | 0.19          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB2 | 18       | 0.18          |
| (1,2077) | 1:103:A:SER:H   | 1:103:A:SER:HB3 | 18       | 0.18          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2 | 11       | 0.18          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3 | 11       | 0.18          |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG2 | 9        | 0.18          |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG3 | 9        | 0.18          |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG2 | 9        | 0.18          |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG3 | 9        | 0.18          |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG2 | 9        | 0.18          |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG3 | 9        | 0.18          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11 | 16       | 0.18          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12 | 16       | 0.18          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13 | 16       | 0.18          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11 | 16       | 0.18          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12 | 16       | 0.18          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13 | 16       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11 | 4        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12 | 4        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13 | 4        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21 | 4        | 0.18          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 4        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 4        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11  | 6        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12  | 6        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 6        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 6        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 6        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 6        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11  | 9        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12  | 9        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 9        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 9        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 9        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 9        | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11  | 13       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12  | 13       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 13       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 13       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 13       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 13       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG11  | 19       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG12  | 19       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG13  | 19       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG21  | 19       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG22  | 19       | 0.18          |
| (1,1906) | 1:26:A:MET:HB2 | 1:27:A:VAL:HG23  | 19       | 0.18          |
| (1,1861) | 1:11:A:LYS:HE2 | 1:48:A:PRO:HD2   | 20       | 0.18          |
| (1,1861) | 1:11:A:LYS:HE2 | 1:48:A:PRO:HD3   | 20       | 0.18          |
| (1,1861) | 1:11:A:LYS:HE3 | 1:48:A:PRO:HD2   | 20       | 0.18          |
| (1,1861) | 1:11:A:LYS:HE3 | 1:48:A:PRO:HD3   | 20       | 0.18          |
| (1,1802) | 1:66:A:TRP:H   | 1:68:A:LEU:HB3   | 1        | 0.18          |
| (1,1802) | 1:66:A:TRP:H   | 1:68:A:LEU:HB3   | 2        | 0.18          |
| (1,1802) | 1:66:A:TRP:H   | 1:68:A:LEU:HB3   | 4        | 0.18          |
| (1,1802) | 1:66:A:TRP:H   | 1:68:A:LEU:HB3   | 19       | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 4        | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 4        | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 4        | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 5        | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 5        | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG23 | 5        | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG21 | 8        | 0.18          |
| (1,1729) | 1:54:A:THR:H   | 1:112:A:VAL:HG22 | 8        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 8        | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 11       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 11       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 11       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 13       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 13       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 13       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 14       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 14       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 14       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 18       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 18       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 18       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 19       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 19       | 0.18          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 19       | 0.18          |
| (1,1666) | 1:102:A:LYS:HE2 | 1:103:A:SER:H    | 11       | 0.18          |
| (1,1666) | 1:102:A:LYS:HE3 | 1:103:A:SER:H    | 11       | 0.18          |
| (1,1666) | 1:102:A:LYS:HE2 | 1:103:A:SER:H    | 17       | 0.18          |
| (1,1666) | 1:102:A:LYS:HE3 | 1:103:A:SER:H    | 17       | 0.18          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 10       | 0.18          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 15       | 0.18          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 15       | 0.18          |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 10       | 0.18          |
| (1,1383) | 1:94:A:LYS:H    | 1:97:A:LYS:HG3   | 16       | 0.18          |
| (1,1315) | 1:121:A:LYS:H   | 1:121:A:LYS:HG2  | 4        | 0.18          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 5        | 0.18          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 17       | 0.18          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 5        | 0.18          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 18       | 0.18          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 9        | 0.18          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 9        | 0.18          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 9        | 0.18          |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 2        | 0.18          |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 14       | 0.18          |
| (1,898)  | 1:97:A:LYS:H    | 1:97:A:LYS:HG3   | 18       | 0.18          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 5        | 0.18          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 15       | 0.18          |
| (1,618)  | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 8        | 0.18          |
| (1,618)  | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 18       | 0.18          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 2        | 0.18          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 13       | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 19       | 0.18          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 17       | 0.17          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 17       | 0.17          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11  | 11       | 0.17          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12  | 11       | 0.17          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13  | 11       | 0.17          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11  | 11       | 0.17          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12  | 11       | 0.17          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13  | 11       | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11  | 2        | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12  | 2        | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13  | 2        | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21  | 2        | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG22  | 2        | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG23  | 2        | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11  | 20       | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12  | 20       | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13  | 20       | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21  | 20       | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG22  | 20       | 0.17          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG23  | 20       | 0.17          |
| (1,1900) | 1:25:A:LEU:HD11 | 1:87:A:ILE:HG13  | 10       | 0.17          |
| (1,1900) | 1:25:A:LEU:HD12 | 1:87:A:ILE:HG13  | 10       | 0.17          |
| (1,1900) | 1:25:A:LEU:HD13 | 1:87:A:ILE:HG13  | 10       | 0.17          |
| (1,1900) | 1:25:A:LEU:HD21 | 1:87:A:ILE:HG13  | 10       | 0.17          |
| (1,1900) | 1:25:A:LEU:HD22 | 1:87:A:ILE:HG13  | 10       | 0.17          |
| (1,1900) | 1:25:A:LEU:HD23 | 1:87:A:ILE:HG13  | 10       | 0.17          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA2   | 12       | 0.17          |
| (1,1860) | 1:11:A:LYS:HE2  | 1:12:A:GLY:HA3   | 12       | 0.17          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA2   | 12       | 0.17          |
| (1,1860) | 1:11:A:LYS:HE3  | 1:12:A:GLY:HA3   | 12       | 0.17          |
| (1,1845) | 1:9:A:TYR:HB2   | 1:10:A:LYS:H     | 10       | 0.17          |
| (1,1845) | 1:9:A:TYR:HB3   | 1:10:A:LYS:H     | 10       | 0.17          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 13       | 0.17          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3   | 14       | 0.17          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG21 | 17       | 0.17          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG22 | 17       | 0.17          |
| (1,1729) | 1:54:A:THR:H    | 1:112:A:VAL:HG23 | 17       | 0.17          |
| (1,1666) | 1:102:A:LYS:HE2 | 1:103:A:SER:H    | 10       | 0.17          |
| (1,1666) | 1:102:A:LYS:HE3 | 1:103:A:SER:H    | 10       | 0.17          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 5        | 0.17          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 14       | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H    | 18       | 0.17          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 12       | 0.17          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 12       | 0.17          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 4        | 0.17          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 1        | 0.17          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 8        | 0.17          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 10       | 0.17          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 14       | 0.17          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 16       | 0.17          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 11       | 0.17          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 16       | 0.17          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 6        | 0.17          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 6        | 0.17          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 6        | 0.17          |
| (1,806)  | 1:77:A:ARG:HA   | 1:136:A:LYS:HG3  | 1        | 0.17          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 4        | 0.17          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 9        | 0.17          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 10       | 0.17          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 19       | 0.17          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 2        | 0.17          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 2        | 0.17          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 2        | 0.17          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 8        | 0.17          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 8        | 0.17          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 8        | 0.17          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 3        | 0.17          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 9        | 0.17          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 12       | 0.17          |
| (1,680)  | 1:72:A:ALA:HA   | 1:76:A:PHE:HB2   | 4        | 0.17          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H    | 11       | 0.17          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H    | 12       | 0.17          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 12       | 0.17          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 12       | 0.17          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 9        | 0.17          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 9        | 0.17          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 9        | 0.17          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 4        | 0.17          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 1        | 0.17          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 2        | 0.17          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 4        | 0.17          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 6        | 0.17          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 9        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2 | 12       | 0.17          |
| (1,113)  | 1:68:A:LEU:HD21 | 1:78:A:VAL:HB   | 4        | 0.17          |
| (1,113)  | 1:68:A:LEU:HD22 | 1:78:A:VAL:HB   | 4        | 0.17          |
| (1,113)  | 1:68:A:LEU:HD23 | 1:78:A:VAL:HB   | 4        | 0.17          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 11       | 0.17          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 20       | 0.17          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2 | 14       | 0.16          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3 | 14       | 0.16          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2 | 7        | 0.16          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3 | 7        | 0.16          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2 | 7        | 0.16          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3 | 7        | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11 | 9        | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12 | 9        | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13 | 9        | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11 | 9        | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12 | 9        | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13 | 9        | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11 | 15       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12 | 15       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13 | 15       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11 | 15       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12 | 15       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13 | 15       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11 | 18       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12 | 18       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13 | 18       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11 | 18       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12 | 18       | 0.16          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13 | 18       | 0.16          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3  | 8        | 0.16          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3  | 10       | 0.16          |
| (1,1802) | 1:66:A:TRP:H    | 1:68:A:LEU:HB3  | 17       | 0.16          |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H    | 4        | 0.16          |
| (1,1666) | 1:102:A:LYS:HE2 | 1:103:A:SER:H   | 5        | 0.16          |
| (1,1666) | 1:102:A:LYS:HE3 | 1:103:A:SER:H   | 5        | 0.16          |
| (1,1666) | 1:102:A:LYS:HE2 | 1:103:A:SER:H   | 14       | 0.16          |
| (1,1666) | 1:102:A:LYS:HE3 | 1:103:A:SER:H   | 14       | 0.16          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3  | 3        | 0.16          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3  | 15       | 0.16          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3  | 18       | 0.16          |
| (1,1481) | 1:87:A:ILE:HA   | 1:126:A:ASN:H   | 16       | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 19       | 0.16          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 20       | 0.16          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 20       | 0.16          |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA    | 11       | 0.16          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 20       | 0.16          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 20       | 0.16          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 20       | 0.16          |
| (1,1191) | 1:78:A:VAL:HG11 | 1:80:A:GLU:H     | 5        | 0.16          |
| (1,1191) | 1:78:A:VAL:HG12 | 1:80:A:GLU:H     | 5        | 0.16          |
| (1,1191) | 1:78:A:VAL:HG13 | 1:80:A:GLU:H     | 5        | 0.16          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 6        | 0.16          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 9        | 0.16          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 19       | 0.16          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 20       | 0.16          |
| (1,1033) | 1:118:A:GLU:H   | 1:118:A:GLU:HB3  | 10       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 2        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 2        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 2        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 4        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 4        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 4        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 7        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 7        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 7        | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 12       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 12       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 12       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 13       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 13       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 13       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 20       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 20       | 0.16          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 20       | 0.16          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 9        | 0.16          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 9        | 0.16          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 15       | 0.16          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 15       | 0.16          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 1        | 0.16          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 2        | 0.16          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 11       | 0.16          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 17       | 0.16          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 4        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22 | 4        | 0.16          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23 | 4        | 0.16          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 1        | 0.16          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 6        | 0.16          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 11       | 0.16          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2 | 17       | 0.16          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H   | 15       | 0.16          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H   | 16       | 0.16          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H   | 18       | 0.16          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2  | 4        | 0.16          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3  | 4        | 0.16          |
| (1,483)  | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 1        | 0.16          |
| (1,483)  | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 1        | 0.16          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2 | 15       | 0.16          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2 | 3        | 0.16          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2 | 7        | 0.16          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2 | 13       | 0.16          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2 | 19       | 0.16          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2 | 20       | 0.16          |
| (1,2150) | 1:135:A:LYS:HB2 | 1:136:A:LYS:HE2 | 13       | 0.15          |
| (1,2150) | 1:135:A:LYS:HB2 | 1:136:A:LYS:HE3 | 13       | 0.15          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11 | 20       | 0.15          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12 | 20       | 0.15          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13 | 20       | 0.15          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11 | 20       | 0.15          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12 | 20       | 0.15          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13 | 20       | 0.15          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG11 | 7        | 0.15          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG12 | 7        | 0.15          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG13 | 7        | 0.15          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG21 | 7        | 0.15          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG22 | 7        | 0.15          |
| (1,1906) | 1:26:A:MET:HB2  | 1:27:A:VAL:HG23 | 7        | 0.15          |
| (1,1850) | 1:10:A:LYS:HB2  | 1:62:A:TYR:HE1  | 18       | 0.15          |
| (1,1850) | 1:10:A:LYS:HB3  | 1:62:A:TYR:HE1  | 18       | 0.15          |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H    | 5        | 0.15          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1  | 4        | 0.15          |
| (1,1666) | 1:102:A:LYS:HE2 | 1:103:A:SER:H   | 18       | 0.15          |
| (1,1666) | 1:102:A:LYS:HE3 | 1:103:A:SER:H   | 18       | 0.15          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H   | 13       | 0.15          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2  | 14       | 0.15          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2  | 15       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 16       | 0.15          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 8        | 0.15          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 8        | 0.15          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 8        | 0.15          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 13       | 0.15          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 11       | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 1        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 1        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 1        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 3        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 3        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 3        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 8        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 8        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 8        | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 15       | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 15       | 0.15          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 15       | 0.15          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 6        | 0.15          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 6        | 0.15          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 12       | 0.15          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 12       | 0.15          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 18       | 0.15          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 18       | 0.15          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 12       | 0.15          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 14       | 0.15          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 18       | 0.15          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 20       | 0.15          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 3        | 0.15          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 3        | 0.15          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 3        | 0.15          |
| (1,618)  | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 15       | 0.15          |
| (1,483)  | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 6        | 0.15          |
| (1,483)  | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 6        | 0.15          |
| (1,483)  | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 12       | 0.15          |
| (1,483)  | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 12       | 0.15          |
| (1,434)  | 1:10:A:LYS:HD2  | 1:62:A:TYR:HE1   | 12       | 0.15          |
| (1,434)  | 1:10:A:LYS:HD3  | 1:62:A:TYR:HE1   | 12       | 0.15          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 10       | 0.15          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 10       | 0.15          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 10       | 0.15          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 5        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 11       | 0.15          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 20       | 0.15          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 8        | 0.15          |
| (1,214)  | 1:88:A:GLU:HA   | 1:103:A:SER:HB2  | 15       | 0.15          |
| (1,132)  | 1:121:A:LYS:HA  | 1:121:A:LYS:HB2  | 15       | 0.15          |
| (1,2148) | 1:135:A:LYS:HA  | 1:136:A:LYS:HD2  | 6        | 0.14          |
| (1,2148) | 1:135:A:LYS:HA  | 1:136:A:LYS:HD3  | 6        | 0.14          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 15       | 0.14          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 15       | 0.14          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 15       | 0.14          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 15       | 0.14          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 15       | 0.14          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 15       | 0.14          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 7        | 0.14          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 7        | 0.14          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11  | 12       | 0.14          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12  | 12       | 0.14          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13  | 12       | 0.14          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11  | 12       | 0.14          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12  | 12       | 0.14          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13  | 12       | 0.14          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 4        | 0.14          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 5        | 0.14          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 8        | 0.14          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 12       | 0.14          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3   | 6        | 0.14          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3   | 11       | 0.14          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 2        | 0.14          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 10       | 0.14          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 6        | 0.14          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 6        | 0.14          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 9        | 0.14          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 9        | 0.14          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2   | 1        | 0.14          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3   | 1        | 0.14          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB2   | 8        | 0.14          |
| (1,1353) | 1:74:A:LYS:H    | 1:74:A:LYS:HB3   | 8        | 0.14          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 1        | 0.14          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 12       | 0.14          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 1        | 0.14          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 3        | 0.14          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 2        | 0.14          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 13       | 0.14          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 5        | 0.14          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 7        | 0.14          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 16       | 0.14          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 20       | 0.14          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 5        | 0.14          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 5        | 0.14          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 5        | 0.14          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 19       | 0.14          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 19       | 0.14          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 19       | 0.14          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 16       | 0.14          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 16       | 0.14          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 3        | 0.14          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 6        | 0.14          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 8        | 0.14          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG21  | 1        | 0.14          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG22  | 1        | 0.14          |
| (1,698)  | 1:68:A:LEU:HB2  | 1:78:A:VAL:HG23  | 1        | 0.14          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 14       | 0.14          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 18       | 0.14          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 12       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 1        | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 1        | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 1        | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 4        | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 4        | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 4        | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 12       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 12       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 12       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 14       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 14       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 14       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 17       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 17       | 0.14          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 17       | 0.14          |
| (1,618)  | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 20       | 0.14          |
| (1,608)  | 1:76:A:PHE:HA   | 1:134:A:GLU:H    | 20       | 0.14          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 1        | 0.14          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 1        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,511) | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2  | 5        | 0.14          |
| (1,511) | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3  | 5        | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 2        | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 2        | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 3        | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 3        | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 4        | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 4        | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 9        | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 9        | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 10       | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 10       | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 11       | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 11       | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 13       | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 13       | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 14       | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 14       | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 17       | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 17       | 0.14          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA  | 19       | 0.14          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA  | 19       | 0.14          |
| (1,379) | 1:28:A:ASN:H    | 1:126:A:ASN:HA  | 1        | 0.14          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1 | 14       | 0.14          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1 | 14       | 0.14          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1 | 14       | 0.14          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1 | 17       | 0.14          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1 | 17       | 0.14          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1 | 17       | 0.14          |
| (1,351) | 1:67:A:ALA:HB1  | 1:71:A:THR:HB   | 8        | 0.14          |
| (1,351) | 1:67:A:ALA:HB2  | 1:71:A:THR:HB   | 8        | 0.14          |
| (1,351) | 1:67:A:ALA:HB3  | 1:71:A:THR:HB   | 8        | 0.14          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 17       | 0.14          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 17       | 0.14          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 17       | 0.14          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 20       | 0.14          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 20       | 0.14          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 20       | 0.14          |
| (1,266) | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2 | 7        | 0.14          |
| (1,266) | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2 | 14       | 0.14          |
| (1,266) | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2 | 17       | 0.14          |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H    | 7        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB1   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB2   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB3   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB1   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB2   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB3   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB1   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB2   | 7        | 0.14          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB3   | 7        | 0.14          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 8        | 0.13          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 8        | 0.13          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 8        | 0.13          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 8        | 0.13          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 8        | 0.13          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 8        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 1        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 1        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 2        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 2        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 4        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 4        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 8        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 8        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 9        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 9        | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 12       | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 12       | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 13       | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 13       | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 19       | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 19       | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 20       | 0.13          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 20       | 0.13          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 9        | 0.13          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 9        | 0.13          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 9        | 0.13          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 9        | 0.13          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11  | 8        | 0.13          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12  | 8        | 0.13          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13  | 8        | 0.13          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11  | 8        | 0.13          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12  | 8        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1996) | 1:77:A:ARG:HD3 | 1:79:A:VAL:HG13 | 8        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG2 | 1:81:A:LEU:HD11 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG2 | 1:81:A:LEU:HD12 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG2 | 1:81:A:LEU:HD13 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG2 | 1:81:A:LEU:HD21 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG2 | 1:81:A:LEU:HD22 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG2 | 1:81:A:LEU:HD23 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG3 | 1:81:A:LEU:HD11 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG3 | 1:81:A:LEU:HD12 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG3 | 1:81:A:LEU:HD13 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG3 | 1:81:A:LEU:HD21 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG3 | 1:81:A:LEU:HD22 | 9        | 0.13          |
| (1,1981) | 1:61:A:GLU:HG3 | 1:81:A:LEU:HD23 | 9        | 0.13          |
| (1,1802) | 1:66:A:TRP:H   | 1:68:A:LEU:HB3  | 7        | 0.13          |
| (1,1762) | 1:33:A:ASP:H   | 1:39:A:LEU:HB3  | 3        | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 1        | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 6        | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 7        | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 10       | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 14       | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 16       | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 18       | 0.13          |
| (1,1745) | 1:61:A:GLU:H   | 1:63:A:TYR:HB2  | 20       | 0.13          |
| (1,1738) | 1:47:A:PHE:HA  | 1:49:A:ILE:H    | 1        | 0.13          |
| (1,1738) | 1:47:A:PHE:HA  | 1:49:A:ILE:H    | 13       | 0.13          |
| (1,1664) | 1:88:A:GLU:H   | 1:126:A:ASN:HB3 | 9        | 0.13          |
| (1,1653) | 1:60:A:ILE:H   | 1:63:A:TYR:HB2  | 4        | 0.13          |
| (1,1580) | 1:26:A:MET:H   | 1:46:A:GLU:HB3  | 1        | 0.13          |
| (1,1580) | 1:26:A:MET:H   | 1:46:A:GLU:HB3  | 5        | 0.13          |
| (1,1580) | 1:26:A:MET:H   | 1:46:A:GLU:HB3  | 14       | 0.13          |
| (1,1580) | 1:26:A:MET:H   | 1:46:A:GLU:HB3  | 17       | 0.13          |
| (1,1475) | 1:31:A:GLY:H   | 1:130:A:LYS:HA  | 4        | 0.13          |
| (1,1432) | 1:25:A:LEU:HB2 | 1:125:A:PHE:H   | 4        | 0.13          |
| (1,1432) | 1:25:A:LEU:HB2 | 1:125:A:PHE:H   | 6        | 0.13          |
| (1,1432) | 1:25:A:LEU:HB2 | 1:125:A:PHE:H   | 7        | 0.13          |
| (1,1432) | 1:25:A:LEU:HB2 | 1:125:A:PHE:H   | 20       | 0.13          |
| (1,1407) | 1:47:A:PHE:HE1 | 1:66:A:TRP:H    | 7        | 0.13          |
| (1,1407) | 1:47:A:PHE:HE2 | 1:66:A:TRP:H    | 7        | 0.13          |
| (1,1407) | 1:47:A:PHE:HE1 | 1:66:A:TRP:H    | 8        | 0.13          |
| (1,1407) | 1:47:A:PHE:HE2 | 1:66:A:TRP:H    | 8        | 0.13          |
| (1,1407) | 1:47:A:PHE:HE1 | 1:66:A:TRP:H    | 18       | 0.13          |
| (1,1407) | 1:47:A:PHE:HE2 | 1:66:A:TRP:H    | 18       | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1392) | 1:109:A:LYS:H   | 1:109:A:LYS:HG2  | 19       | 0.13          |
| (1,1392) | 1:109:A:LYS:H   | 1:109:A:LYS:HG3  | 19       | 0.13          |
| (1,1303) | 1:96:A:LYS:H    | 1:96:A:LYS:HG2   | 18       | 0.13          |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 12       | 0.13          |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA    | 10       | 0.13          |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA    | 16       | 0.13          |
| (1,1281) | 1:61:A:GLU:HB2  | 1:62:A:TYR:H     | 9        | 0.13          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 3        | 0.13          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 4        | 0.13          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 6        | 0.13          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 9        | 0.13          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 13       | 0.13          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 15       | 0.13          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 19       | 0.13          |
| (1,1191) | 1:78:A:VAL:HG11 | 1:80:A:GLU:H     | 6        | 0.13          |
| (1,1191) | 1:78:A:VAL:HG12 | 1:80:A:GLU:H     | 6        | 0.13          |
| (1,1191) | 1:78:A:VAL:HG13 | 1:80:A:GLU:H     | 6        | 0.13          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 2        | 0.13          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H    | 14       | 0.13          |
| (1,1173) | 1:26:A:MET:HB2  | 1:27:A:VAL:H     | 4        | 0.13          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 3        | 0.13          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 6        | 0.13          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 14       | 0.13          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 15       | 0.13          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 16       | 0.13          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 16       | 0.13          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 16       | 0.13          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 17       | 0.13          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 17       | 0.13          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 17       | 0.13          |
| (1,792)  | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 5        | 0.13          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 11       | 0.13          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 11       | 0.13          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE1   | 20       | 0.13          |
| (1,787)  | 1:40:A:LEU:HA   | 1:76:A:PHE:HE2   | 20       | 0.13          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 16       | 0.13          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 5        | 0.13          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 6        | 0.13          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 9        | 0.13          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 11       | 0.13          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 15       | 0.13          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 16       | 0.13          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,671) | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 20       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 2        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 2        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 2        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 3        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 3        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 3        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 5        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 5        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 5        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 6        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 6        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 6        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 9        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 9        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 9        | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 11       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 11       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 11       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 13       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 13       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 13       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 16       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 16       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 16       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 20       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 20       | 0.13          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 20       | 0.13          |
| (1,618) | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 7        | 0.13          |
| (1,618) | 1:55:A:LEU:HB2  | 1:59:A:LYS:HB3   | 9        | 0.13          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 7        | 0.13          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 7        | 0.13          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 8        | 0.13          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 8        | 0.13          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 20       | 0.13          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 20       | 0.13          |
| (1,458) | 1:40:A:LEU:HG   | 1:68:A:LEU:HB3   | 5        | 0.13          |
| (1,428) | 1:26:A:MET:HA   | 1:127:A:LEU:H    | 15       | 0.13          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1  | 5        | 0.13          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1  | 5        | 0.13          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1  | 5        | 0.13          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1  | 18       | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,371)  | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1  | 18       | 0.13          |
| (1,371)  | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1  | 18       | 0.13          |
| (1,351)  | 1:67:A:ALA:HB1  | 1:71:A:THR:HB    | 12       | 0.13          |
| (1,351)  | 1:67:A:ALA:HB2  | 1:71:A:THR:HB    | 12       | 0.13          |
| (1,351)  | 1:67:A:ALA:HB3  | 1:71:A:THR:HB    | 12       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 12       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 12       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 12       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 14       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 14       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 14       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 18       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 18       | 0.13          |
| (1,319)  | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 18       | 0.13          |
| (1,266)  | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 12       | 0.13          |
| (1,213)  | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 1        | 0.13          |
| (1,213)  | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 9        | 0.13          |
| (1,213)  | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 15       | 0.13          |
| (1,213)  | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 18       | 0.13          |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE1   | 9        | 0.13          |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE2   | 9        | 0.13          |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE3   | 9        | 0.13          |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE1   | 12       | 0.13          |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE2   | 12       | 0.13          |
| (1,152)  | 1:26:A:MET:HB2  | 1:26:A:MET:HE3   | 12       | 0.13          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 14       | 0.13          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 15       | 0.13          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 18       | 0.13          |
| (1,67)   | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 17       | 0.13          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 3        | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 3        | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 3        | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 3        | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 3        | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 3        | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 9        | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 9        | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 9        | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 9        | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 9        | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 9        | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 12       | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 12       | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 12       | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 12       | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 12       | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 12       | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 20       | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 20       | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 20       | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 20       | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 20       | 0.12          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 20       | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 3        | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 3        | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 6        | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 6        | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 15       | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 15       | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB2  | 16       | 0.12          |
| (1,2075) | 1:102:A:LYS:HA  | 1:103:A:SER:HB3  | 16       | 0.12          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 6        | 0.12          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 6        | 0.12          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 6        | 0.12          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 6        | 0.12          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 13       | 0.12          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 13       | 0.12          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 13       | 0.12          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 13       | 0.12          |
| (1,1856) | 1:11:A:LYS:HB2  | 1:48:A:PRO:HD2   | 2        | 0.12          |
| (1,1856) | 1:11:A:LYS:HB2  | 1:48:A:PRO:HD3   | 2        | 0.12          |
| (1,1856) | 1:11:A:LYS:HB3  | 1:48:A:PRO:HD2   | 2        | 0.12          |
| (1,1856) | 1:11:A:LYS:HB3  | 1:48:A:PRO:HD3   | 2        | 0.12          |
| (1,1850) | 1:10:A:LYS:HB2  | 1:62:A:TYR:HE1   | 20       | 0.12          |
| (1,1850) | 1:10:A:LYS:HB3  | 1:62:A:TYR:HE1   | 20       | 0.12          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 1        | 0.12          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 7        | 0.12          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 3        | 0.12          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 11       | 0.12          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 12       | 0.12          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 13       | 0.12          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 19       | 0.12          |
| (1,1739) | 1:31:A:GLY:HA3  | 1:41:A:SER:H     | 7        | 0.12          |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H     | 2        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 1        | 0.12          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 9        | 0.12          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 11       | 0.12          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 13       | 0.12          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 15       | 0.12          |
| (1,1700) | 1:21:A:THR:HG21 | 1:122:A:ASN:HD22 | 4        | 0.12          |
| (1,1700) | 1:21:A:THR:HG22 | 1:122:A:ASN:HD22 | 4        | 0.12          |
| (1,1700) | 1:21:A:THR:HG23 | 1:122:A:ASN:HD22 | 4        | 0.12          |
| (1,1664) | 1:88:A:GLU:H    | 1:126:A:ASN:HB3  | 6        | 0.12          |
| (1,1641) | 1:51:A:PRO:HB2  | 1:116:A:LEU:H    | 19       | 0.12          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3   | 9        | 0.12          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3   | 12       | 0.12          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 8        | 0.12          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 12       | 0.12          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 16       | 0.12          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 11       | 0.12          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 11       | 0.12          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 16       | 0.12          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 16       | 0.12          |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 8        | 0.12          |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA    | 20       | 0.12          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 2        | 0.12          |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2  | 8        | 0.12          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 4        | 0.12          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 4        | 0.12          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 4        | 0.12          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 7        | 0.12          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 7        | 0.12          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 7        | 0.12          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 16       | 0.12          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 16       | 0.12          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 16       | 0.12          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H    | 19       | 0.12          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H    | 19       | 0.12          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H    | 19       | 0.12          |
| (1,1185) | 1:90:A:THR:HG21 | 1:91:A:TYR:H     | 4        | 0.12          |
| (1,1185) | 1:90:A:THR:HG22 | 1:91:A:TYR:H     | 4        | 0.12          |
| (1,1185) | 1:90:A:THR:HG23 | 1:91:A:TYR:H     | 4        | 0.12          |
| (1,1185) | 1:90:A:THR:HG21 | 1:91:A:TYR:H     | 6        | 0.12          |
| (1,1185) | 1:90:A:THR:HG22 | 1:91:A:TYR:H     | 6        | 0.12          |
| (1,1185) | 1:90:A:THR:HG23 | 1:91:A:TYR:H     | 6        | 0.12          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 9        | 0.12          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 12       | 0.12          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB   | 17       | 0.12          |
| (1,1130) | 1:25:A:LEU:H    | 1:49:A:ILE:H     | 3        | 0.12          |
| (1,1130) | 1:25:A:LEU:H    | 1:49:A:ILE:H     | 15       | 0.12          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG21 | 11       | 0.12          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG22 | 11       | 0.12          |
| (1,931)  | 1:28:A:ASN:HD22 | 1:128:A:ILE:HG23 | 11       | 0.12          |
| (1,792)  | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 18       | 0.12          |
| (1,749)  | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 7        | 0.12          |
| (1,743)  | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 2        | 0.12          |
| (1,743)  | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 2        | 0.12          |
| (1,743)  | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 13       | 0.12          |
| (1,743)  | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 13       | 0.12          |
| (1,743)  | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 15       | 0.12          |
| (1,743)  | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 15       | 0.12          |
| (1,743)  | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 20       | 0.12          |
| (1,743)  | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 20       | 0.12          |
| (1,683)  | 1:88:A:GLU:H    | 1:126:A:ASN:HB2  | 5        | 0.12          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 8        | 0.12          |
| (1,671)  | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 18       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 7        | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 7        | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 7        | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 10       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 10       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 10       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 15       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 15       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 15       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 18       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 18       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 18       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 19       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 19       | 0.12          |
| (1,620)  | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 19       | 0.12          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG2   | 20       | 0.12          |
| (1,511)  | 1:11:A:LYS:HA   | 1:48:A:PRO:HG3   | 20       | 0.12          |
| (1,507)  | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD11 | 8        | 0.12          |
| (1,507)  | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD12 | 8        | 0.12          |
| (1,507)  | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD13 | 8        | 0.12          |
| (1,507)  | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD11 | 20       | 0.12          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD12 | 20       | 0.12          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD13 | 20       | 0.12          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 15       | 0.12          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 15       | 0.12          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 16       | 0.12          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 16       | 0.12          |
| (1,483) | 1:88:A:GLU:HB2  | 1:101:A:THR:HA   | 18       | 0.12          |
| (1,483) | 1:88:A:GLU:HB3  | 1:101:A:THR:HA   | 18       | 0.12          |
| (1,428) | 1:26:A:MET:HA   | 1:127:A:LEU:H    | 11       | 0.12          |
| (1,428) | 1:26:A:MET:HA   | 1:127:A:LEU:H    | 18       | 0.12          |
| (1,379) | 1:28:A:ASN:H    | 1:126:A:ASN:HA   | 5        | 0.12          |
| (1,379) | 1:28:A:ASN:H    | 1:126:A:ASN:HA   | 11       | 0.12          |
| (1,379) | 1:28:A:ASN:H    | 1:126:A:ASN:HA   | 18       | 0.12          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1  | 10       | 0.12          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1  | 10       | 0.12          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1  | 10       | 0.12          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1  | 11       | 0.12          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1  | 11       | 0.12          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1  | 11       | 0.12          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB    | 3        | 0.12          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB    | 3        | 0.12          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB    | 3        | 0.12          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB    | 12       | 0.12          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB    | 12       | 0.12          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB    | 12       | 0.12          |
| (1,281) | 1:10:A:LYS:HA   | 1:11:A:LYS:H     | 7        | 0.12          |
| (1,266) | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 1        | 0.12          |
| (1,266) | 1:28:A:ASN:HB3  | 1:126:A:ASN:HB2  | 6        | 0.12          |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 2        | 0.12          |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 4        | 0.12          |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H     | 13       | 0.12          |
| (1,113) | 1:68:A:LEU:HD21 | 1:78:A:VAL:HB    | 3        | 0.12          |
| (1,113) | 1:68:A:LEU:HD22 | 1:78:A:VAL:HB    | 3        | 0.12          |
| (1,113) | 1:68:A:LEU:HD23 | 1:78:A:VAL:HB    | 3        | 0.12          |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 7        | 0.12          |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 17       | 0.12          |
| (1,67)  | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 1        | 0.12          |
| (1,67)  | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 2        | 0.12          |
| (1,67)  | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 3        | 0.12          |
| (1,67)  | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 5        | 0.12          |
| (1,67)  | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 6        | 0.12          |
| (1,67)  | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 11       | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,67)   | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 12       | 0.12          |
| (1,67)   | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 13       | 0.12          |
| (1,67)   | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 14       | 0.12          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB1   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB2   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB3   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB1   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB2   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB3   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB1   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB2   | 2        | 0.12          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB3   | 2        | 0.12          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 2        | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 2        | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 2        | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 2        | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 2        | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 2        | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 7        | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 7        | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 7        | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 7        | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 7        | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 7        | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 19       | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 19       | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 19       | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 19       | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 19       | 0.11          |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 19       | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 1        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 1        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 1        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 1        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 2        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 2        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 2        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 2        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 4        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 4        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 4        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 4        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 8        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 8        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 8        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 8        | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 15       | 0.11          |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 15       | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 15       | 0.11          |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 15       | 0.11          |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG2  | 6        | 0.11          |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG3  | 6        | 0.11          |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG2  | 6        | 0.11          |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG3  | 6        | 0.11          |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG2  | 6        | 0.11          |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG3  | 6        | 0.11          |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG2  | 13       | 0.11          |
| (1,2000) | 1:79:A:VAL:HG11 | 1:134:A:GLU:HG3  | 13       | 0.11          |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG2  | 13       | 0.11          |
| (1,2000) | 1:79:A:VAL:HG12 | 1:134:A:GLU:HG3  | 13       | 0.11          |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG2  | 13       | 0.11          |
| (1,2000) | 1:79:A:VAL:HG13 | 1:134:A:GLU:HG3  | 13       | 0.11          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG11  | 13       | 0.11          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG12  | 13       | 0.11          |
| (1,1996) | 1:77:A:ARG:HD2  | 1:79:A:VAL:HG13  | 13       | 0.11          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG11  | 13       | 0.11          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG12  | 13       | 0.11          |
| (1,1996) | 1:77:A:ARG:HD3  | 1:79:A:VAL:HG13  | 13       | 0.11          |
| (1,1805) | 1:79:A:VAL:H    | 1:133:A:ILE:HD11 | 7        | 0.11          |
| (1,1805) | 1:79:A:VAL:H    | 1:133:A:ILE:HD12 | 7        | 0.11          |
| (1,1805) | 1:79:A:VAL:H    | 1:133:A:ILE:HD13 | 7        | 0.11          |
| (1,1779) | 1:59:A:LYS:HB2  | 1:63:A:TYR:H     | 9        | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 2        | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 4        | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 5        | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 6        | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 8        | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 10       | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 12       | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 13       | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 14       | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 16       | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 17       | 0.11          |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3   | 19       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 2        | 0.11          |
| (1,1745) | 1:61:A:GLU:H    | 1:63:A:TYR:HB2   | 15       | 0.11          |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H     | 6        | 0.11          |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H     | 7        | 0.11          |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H     | 18       | 0.11          |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H     | 19       | 0.11          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 6        | 0.11          |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1   | 18       | 0.11          |
| (1,1695) | 1:44:A:TYR:HD1  | 1:46:A:GLU:H     | 16       | 0.11          |
| (1,1664) | 1:88:A:GLU:H    | 1:126:A:ASN:HB3  | 1        | 0.11          |
| (1,1664) | 1:88:A:GLU:H    | 1:126:A:ASN:HB3  | 12       | 0.11          |
| (1,1657) | 1:125:A:PHE:HD1 | 1:126:A:ASN:H    | 9        | 0.11          |
| (1,1657) | 1:125:A:PHE:HD1 | 1:126:A:ASN:H    | 20       | 0.11          |
| (1,1653) | 1:60:A:ILE:H    | 1:63:A:TYR:HB2   | 1        | 0.11          |
| (1,1641) | 1:51:A:PRO:HB2  | 1:116:A:LEU:H    | 2        | 0.11          |
| (1,1641) | 1:51:A:PRO:HB2  | 1:116:A:LEU:H    | 3        | 0.11          |
| (1,1641) | 1:51:A:PRO:HB2  | 1:116:A:LEU:H    | 13       | 0.11          |
| (1,1641) | 1:51:A:PRO:HB2  | 1:116:A:LEU:H    | 15       | 0.11          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3   | 2        | 0.11          |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3   | 19       | 0.11          |
| (1,1541) | 1:20:A:PRO:HG3  | 1:122:A:ASN:HD21 | 8        | 0.11          |
| (1,1485) | 1:65:A:GLU:HG3  | 1:66:A:TRP:H     | 3        | 0.11          |
| (1,1475) | 1:31:A:GLY:H    | 1:130:A:LYS:HA   | 1        | 0.11          |
| (1,1475) | 1:31:A:GLY:H    | 1:130:A:LYS:HA   | 2        | 0.11          |
| (1,1475) | 1:31:A:GLY:H    | 1:130:A:LYS:HA   | 14       | 0.11          |
| (1,1475) | 1:31:A:GLY:H    | 1:130:A:LYS:HA   | 17       | 0.11          |
| (1,1447) | 1:79:A:VAL:H    | 1:80:A:GLU:HG2   | 10       | 0.11          |
| (1,1447) | 1:79:A:VAL:H    | 1:80:A:GLU:HG3   | 10       | 0.11          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 1        | 0.11          |
| (1,1432) | 1:25:A:LEU:HB2  | 1:125:A:PHE:H    | 9        | 0.11          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 5        | 0.11          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 5        | 0.11          |
| (1,1407) | 1:47:A:PHE:HE1  | 1:66:A:TRP:H     | 13       | 0.11          |
| (1,1407) | 1:47:A:PHE:HE2  | 1:66:A:TRP:H     | 13       | 0.11          |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 4        | 0.11          |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 7        | 0.11          |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 9        | 0.11          |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 13       | 0.11          |
| (1,1295) | 1:44:A:TYR:HB2  | 1:45:A:VAL:H     | 20       | 0.11          |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA    | 5        | 0.11          |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA    | 6        | 0.11          |
| (1,1289) | 1:122:A:ASN:HA  | 1:122:A:ASN:HD22 | 4        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2 | 20       | 0.11          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H   | 2        | 0.11          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H   | 2        | 0.11          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H   | 2        | 0.11          |
| (1,1219) | 1:26:A:MET:HE1  | 1:127:A:LEU:H   | 13       | 0.11          |
| (1,1219) | 1:26:A:MET:HE2  | 1:127:A:LEU:H   | 13       | 0.11          |
| (1,1219) | 1:26:A:MET:HE3  | 1:127:A:LEU:H   | 13       | 0.11          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H   | 6        | 0.11          |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H   | 8        | 0.11          |
| (1,1185) | 1:90:A:THR:HG21 | 1:91:A:TYR:H    | 13       | 0.11          |
| (1,1185) | 1:90:A:THR:HG22 | 1:91:A:TYR:H    | 13       | 0.11          |
| (1,1185) | 1:90:A:THR:HG23 | 1:91:A:TYR:H    | 13       | 0.11          |
| (1,1185) | 1:90:A:THR:HG21 | 1:91:A:TYR:H    | 15       | 0.11          |
| (1,1185) | 1:90:A:THR:HG22 | 1:91:A:TYR:H    | 15       | 0.11          |
| (1,1185) | 1:90:A:THR:HG23 | 1:91:A:TYR:H    | 15       | 0.11          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB  | 1        | 0.11          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB  | 2        | 0.11          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB  | 4        | 0.11          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB  | 10       | 0.11          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB  | 13       | 0.11          |
| (1,1131) | 1:52:A:GLY:H    | 1:112:A:VAL:HB  | 18       | 0.11          |
| (1,980)  | 1:79:A:VAL:H    | 1:79:A:VAL:HG11 | 8        | 0.11          |
| (1,980)  | 1:79:A:VAL:H    | 1:79:A:VAL:HG12 | 8        | 0.11          |
| (1,980)  | 1:79:A:VAL:H    | 1:79:A:VAL:HG13 | 8        | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 1        | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 1        | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 1        | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 5        | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 5        | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 5        | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 11       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 11       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 11       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 12       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 12       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 12       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 15       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 15       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 15       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 16       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 16       | 0.11          |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 16       | 0.11          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,837) | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21  | 18       | 0.11          |
| (1,837) | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22  | 18       | 0.11          |
| (1,837) | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23  | 18       | 0.11          |
| (1,792) | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 8        | 0.11          |
| (1,792) | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 10       | 0.11          |
| (1,792) | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 12       | 0.11          |
| (1,749) | 1:33:A:ASP:HB2  | 1:39:A:LEU:HA    | 13       | 0.11          |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 1        | 0.11          |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 1        | 0.11          |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 4        | 0.11          |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 4        | 0.11          |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 6        | 0.11          |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 6        | 0.11          |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 7        | 0.11          |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 7        | 0.11          |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 9        | 0.11          |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 9        | 0.11          |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 12       | 0.11          |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 12       | 0.11          |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 19       | 0.11          |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 19       | 0.11          |
| (1,671) | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 3        | 0.11          |
| (1,671) | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 13       | 0.11          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG21 | 8        | 0.11          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG22 | 8        | 0.11          |
| (1,620) | 1:54:A:THR:HA   | 1:112:A:VAL:HG23 | 8        | 0.11          |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 2        | 0.11          |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 4        | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD11 | 7        | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD12 | 7        | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD13 | 7        | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD11 | 9        | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD12 | 9        | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD13 | 9        | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD11 | 15       | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD12 | 15       | 0.11          |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD13 | 15       | 0.11          |
| (1,475) | 1:102:A:LYS:HB2 | 1:104:A:PHE:HE1  | 3        | 0.11          |
| (1,458) | 1:40:A:LEU:HG   | 1:68:A:LEU:HB3   | 6        | 0.11          |
| (1,458) | 1:40:A:LEU:HG   | 1:68:A:LEU:HB3   | 9        | 0.11          |
| (1,458) | 1:40:A:LEU:HG   | 1:68:A:LEU:HB3   | 18       | 0.11          |
| (1,428) | 1:26:A:MET:HA   | 1:127:A:LEU:H    | 3        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,428) | 1:26:A:MET:HA   | 1:127:A:LEU:H   | 5        | 0.11          |
| (1,395) | 1:102:A:LYS:HB3 | 1:104:A:PHE:HE1 | 10       | 0.11          |
| (1,379) | 1:28:A:ASN:H    | 1:126:A:ASN:HA  | 6        | 0.11          |
| (1,379) | 1:28:A:ASN:H    | 1:126:A:ASN:HA  | 12       | 0.11          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1 | 12       | 0.11          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1 | 12       | 0.11          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1 | 12       | 0.11          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1 | 13       | 0.11          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1 | 13       | 0.11          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1 | 13       | 0.11          |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1 | 16       | 0.11          |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1 | 16       | 0.11          |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1 | 16       | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 1        | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 1        | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 1        | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 2        | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 2        | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 2        | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 4        | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 4        | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 4        | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 6        | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 6        | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 6        | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 7        | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 7        | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 7        | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 8        | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 8        | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 8        | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 9        | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 9        | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 9        | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 13       | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 13       | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 13       | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 19       | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 19       | 0.11          |
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 19       | 0.11          |
| (1,357) | 1:89:A:VAL:HG21 | 1:90:A:THR:HB   | 20       | 0.11          |
| (1,357) | 1:89:A:VAL:HG22 | 1:90:A:THR:HB   | 20       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,357) | 1:89:A:VAL:HG23 | 1:90:A:THR:HB   | 20       | 0.11          |
| (1,351) | 1:67:A:ALA:HB1  | 1:71:A:THR:HB   | 16       | 0.11          |
| (1,351) | 1:67:A:ALA:HB2  | 1:71:A:THR:HB   | 16       | 0.11          |
| (1,351) | 1:67:A:ALA:HB3  | 1:71:A:THR:HB   | 16       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 8        | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 8        | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 8        | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 11       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 11       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 11       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 13       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 13       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 13       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 16       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 16       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 16       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 19       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 19       | 0.11          |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 19       | 0.11          |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H    | 6        | 0.11          |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H    | 19       | 0.11          |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H    | 20       | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE1  | 1        | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE2  | 1        | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE3  | 1        | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE1  | 6        | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE2  | 6        | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE3  | 6        | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE1  | 14       | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE2  | 14       | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE3  | 14       | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE1  | 17       | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE2  | 17       | 0.11          |
| (1,152) | 1:26:A:MET:HB2  | 1:26:A:MET:HE3  | 17       | 0.11          |
| (1,113) | 1:68:A:LEU:HD21 | 1:78:A:VAL:HB   | 8        | 0.11          |
| (1,113) | 1:68:A:LEU:HD22 | 1:78:A:VAL:HB   | 8        | 0.11          |
| (1,113) | 1:68:A:LEU:HD23 | 1:78:A:VAL:HB   | 8        | 0.11          |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 1        | 0.11          |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 3        | 0.11          |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 4        | 0.11          |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 5        | 0.11          |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 6        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 8        | 0.11          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 9        | 0.11          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 10       | 0.11          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 12       | 0.11          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 13       | 0.11          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 16       | 0.11          |
| (1,104)  | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2   | 19       | 0.11          |
| (1,67)   | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 4        | 0.11          |
| (1,67)   | 1:55:A:LEU:HB2  | 1:55:A:LEU:HG    | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB1   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB2   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB3   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB1   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB2   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB3   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB1   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB2   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB3   | 14       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB1   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB2   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB3   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB1   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB2   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB3   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB1   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB2   | 19       | 0.11          |
| (1,31)   | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB3   | 19       | 0.11          |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD11 | 1        | 0.1           |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD12 | 1        | 0.1           |
| (1,2079) | 1:103:A:SER:HB2 | 1:128:A:ILE:HD13 | 1        | 0.1           |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD11 | 1        | 0.1           |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD12 | 1        | 0.1           |
| (1,2079) | 1:103:A:SER:HB3 | 1:128:A:ILE:HD13 | 1        | 0.1           |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 12       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 12       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 12       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 12       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 19       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3  | 19       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2  | 19       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3  | 19       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB2  | 20       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2027) | 1:86:A:LYS:HG2  | 1:103:A:SER:HB3 | 20       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB2 | 20       | 0.1           |
| (1,2027) | 1:86:A:LYS:HG3  | 1:103:A:SER:HB3 | 20       | 0.1           |
| (1,1777) | 1:95:A:ASN:HD21 | 1:97:A:LYS:H    | 10       | 0.1           |
| (1,1777) | 1:95:A:ASN:HD21 | 1:97:A:LYS:H    | 11       | 0.1           |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3  | 9        | 0.1           |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3  | 11       | 0.1           |
| (1,1762) | 1:33:A:ASP:H    | 1:39:A:LEU:HB3  | 15       | 0.1           |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H    | 3        | 0.1           |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H    | 9        | 0.1           |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H    | 11       | 0.1           |
| (1,1738) | 1:47:A:PHE:HA   | 1:49:A:ILE:H    | 15       | 0.1           |
| (1,1733) | 1:134:A:GLU:H   | 1:136:A:LYS:H   | 4        | 0.1           |
| (1,1717) | 1:11:A:LYS:H    | 1:62:A:TYR:HE1  | 3        | 0.1           |
| (1,1657) | 1:125:A:PHE:HD1 | 1:126:A:ASN:H   | 15       | 0.1           |
| (1,1653) | 1:60:A:ILE:H    | 1:63:A:TYR:HB2  | 16       | 0.1           |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3  | 10       | 0.1           |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3  | 13       | 0.1           |
| (1,1580) | 1:26:A:MET:H    | 1:46:A:GLU:HB3  | 20       | 0.1           |
| (1,1519) | 1:79:A:VAL:H    | 1:134:A:GLU:HA  | 13       | 0.1           |
| (1,1447) | 1:79:A:VAL:H    | 1:80:A:GLU:HG2  | 6        | 0.1           |
| (1,1447) | 1:79:A:VAL:H    | 1:80:A:GLU:HG3  | 6        | 0.1           |
| (1,1402) | 1:4:A:PHE:H     | 1:4:A:PHE:HB3   | 20       | 0.1           |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA   | 4        | 0.1           |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA   | 15       | 0.1           |
| (1,1294) | 1:96:A:LYS:H    | 1:97:A:LYS:HA   | 17       | 0.1           |
| (1,1250) | 1:87:A:ILE:H    | 1:104:A:PHE:HB2 | 7        | 0.1           |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H   | 5        | 0.1           |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H   | 12       | 0.1           |
| (1,1186) | 1:130:A:LYS:HB3 | 1:131:A:VAL:H   | 18       | 0.1           |
| (1,1185) | 1:90:A:THR:HG21 | 1:91:A:TYR:H    | 1        | 0.1           |
| (1,1185) | 1:90:A:THR:HG22 | 1:91:A:TYR:H    | 1        | 0.1           |
| (1,1185) | 1:90:A:THR:HG23 | 1:91:A:TYR:H    | 1        | 0.1           |
| (1,1142) | 1:8:A:LYS:HA    | 1:9:A:TYR:H     | 4        | 0.1           |
| (1,895)  | 1:125:A:PHE:H   | 1:125:A:PHE:HD1 | 16       | 0.1           |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 6        | 0.1           |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 6        | 0.1           |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 6        | 0.1           |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 7        | 0.1           |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22 | 7        | 0.1           |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23 | 7        | 0.1           |
| (1,837)  | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG21 | 13       | 0.1           |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,837) | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG22  | 13       | 0.1           |
| (1,837) | 1:63:A:TYR:HB2  | 1:64:A:VAL:HG23  | 13       | 0.1           |
| (1,817) | 1:39:A:LEU:HD11 | 1:135:A:LYS:HA   | 6        | 0.1           |
| (1,817) | 1:39:A:LEU:HD12 | 1:135:A:LYS:HA   | 6        | 0.1           |
| (1,817) | 1:39:A:LEU:HD13 | 1:135:A:LYS:HA   | 6        | 0.1           |
| (1,806) | 1:77:A:ARG:HA   | 1:136:A:LYS:HG3  | 5        | 0.1           |
| (1,792) | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 9        | 0.1           |
| (1,792) | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 11       | 0.1           |
| (1,792) | 1:20:A:PRO:HG3  | 1:122:A:ASN:HB3  | 17       | 0.1           |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 3        | 0.1           |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 3        | 0.1           |
| (1,743) | 1:88:A:GLU:HB2  | 1:103:A:SER:HA   | 8        | 0.1           |
| (1,743) | 1:88:A:GLU:HB3  | 1:103:A:SER:HA   | 8        | 0.1           |
| (1,671) | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 1        | 0.1           |
| (1,671) | 1:37:A:ASN:HD22 | 1:39:A:LEU:HA    | 10       | 0.1           |
| (1,608) | 1:76:A:PHE:HA   | 1:134:A:GLU:H    | 7        | 0.1           |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 7        | 0.1           |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 10       | 0.1           |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 13       | 0.1           |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 16       | 0.1           |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 17       | 0.1           |
| (1,522) | 1:27:A:VAL:H    | 1:126:A:ASN:HA   | 19       | 0.1           |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD11 | 6        | 0.1           |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD12 | 6        | 0.1           |
| (1,507) | 1:87:A:ILE:HG13 | 1:127:A:LEU:HD13 | 6        | 0.1           |
| (1,475) | 1:102:A:LYS:HB2 | 1:104:A:PHE:HE1  | 1        | 0.1           |
| (1,447) | 1:82:A:ASP:HB3  | 1:83:A:PRO:HG2   | 8        | 0.1           |
| (1,447) | 1:82:A:ASP:HB3  | 1:83:A:PRO:HG3   | 8        | 0.1           |
| (1,423) | 1:97:A:LYS:HA   | 1:97:A:LYS:HE3   | 11       | 0.1           |
| (1,423) | 1:97:A:LYS:HA   | 1:97:A:LYS:HE3   | 20       | 0.1           |
| (1,371) | 1:87:A:ILE:HD11 | 1:111:A:PHE:HE1  | 9        | 0.1           |
| (1,371) | 1:87:A:ILE:HD12 | 1:111:A:PHE:HE1  | 9        | 0.1           |
| (1,371) | 1:87:A:ILE:HD13 | 1:111:A:PHE:HE1  | 9        | 0.1           |
| (1,351) | 1:67:A:ALA:HB1  | 1:71:A:THR:HB    | 5        | 0.1           |
| (1,351) | 1:67:A:ALA:HB2  | 1:71:A:THR:HB    | 5        | 0.1           |
| (1,351) | 1:67:A:ALA:HB3  | 1:71:A:THR:HB    | 5        | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 3        | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 3        | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 3        | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21  | 7        | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22  | 7        | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23  | 7        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG21 | 15       | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG22 | 15       | 0.1           |
| (1,319) | 1:50:A:LYS:HG2  | 1:53:A:THR:HG23 | 15       | 0.1           |
| (1,213) | 1:21:A:THR:HB   | 1:22:A:GLY:H    | 5        | 0.1           |
| (1,113) | 1:68:A:LEU:HD21 | 1:78:A:VAL:HB   | 1        | 0.1           |
| (1,113) | 1:68:A:LEU:HD22 | 1:78:A:VAL:HB   | 1        | 0.1           |
| (1,113) | 1:68:A:LEU:HD23 | 1:78:A:VAL:HB   | 1        | 0.1           |
| (1,104) | 1:97:A:LYS:HA   | 1:97:A:LYS:HG2  | 2        | 0.1           |
| (1,31)  | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB1  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB2  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB3  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB1  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB2  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB3  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB1  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB2  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB3  | 10       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB1  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB2  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG11 | 1:67:A:ALA:HB3  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB1  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB2  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG12 | 1:67:A:ALA:HB3  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB1  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB2  | 17       | 0.1           |
| (1,31)  | 1:45:A:VAL:HG13 | 1:67:A:ALA:HB3  | 17       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found