



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 11:19 AM UTC

PDB ID : 7N45 / pdb\_00007n45  
BMRB ID : 50507  
Title : Solution NMR structure of the N-terminal globular domain of the endemic HKU1 coronavirus nucleocapsid protein  
Authors : Caruso, I.P.; Marques, A.L.; Santana-Silva, M.C.; Almeida, F.C.L.; Amorim, G.C.  
Deposited on : 2021-06-03

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

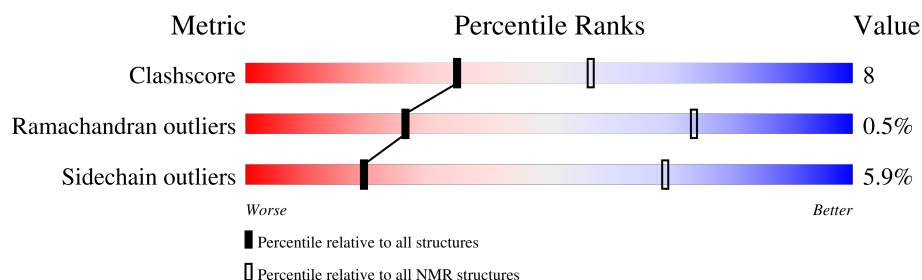
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 138    |                  |

## 2 Ensemble composition and analysis

This entry contains 19 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                            |                   |              |
|--------------------------------------|----------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)      | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:8-A:49, A:64-A:138 (117) | 1.01              | 2            |

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2121 atoms, of which 1020 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleoprotein.

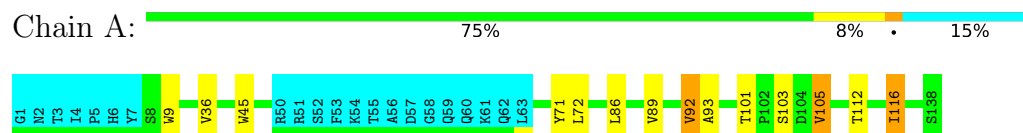
| Mol | Chain | Residues | Atoms |     |      |     |     | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|-------|
| 1   | A     | 138      | Total | C   | H    | N   | O   | 0     |
|     |       |          | 2121  | 705 | 1020 | 189 | 207 |       |

## 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: Nucleoprotein

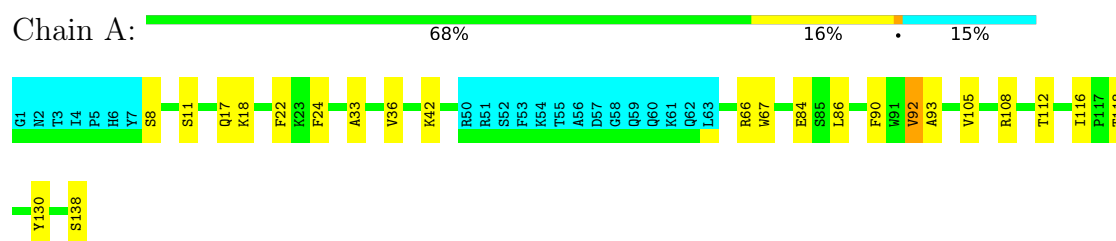


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

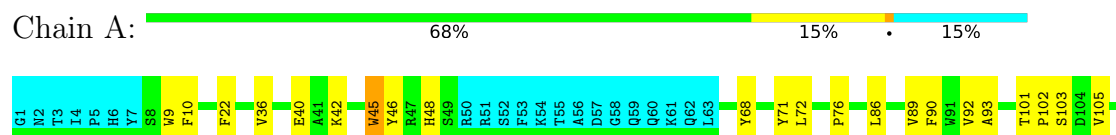
#### 4.2.1 Score per residue for model 1

- Molecule 1: Nucleoprotein



#### 4.2.2 Score per residue for model 2 (medoid)

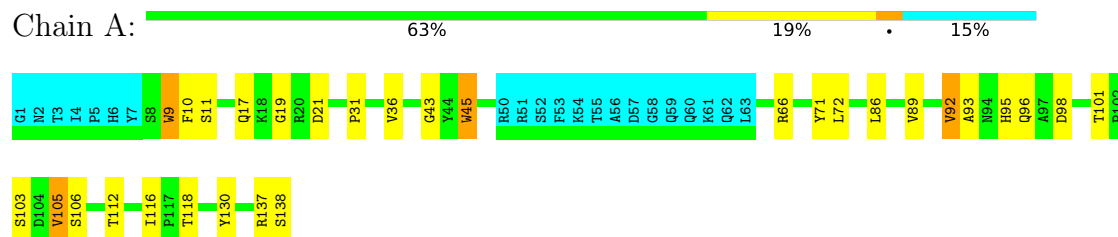
- Molecule 1: Nucleoprotein





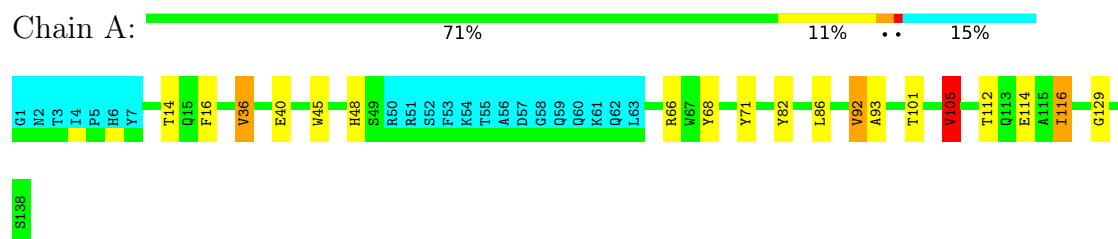
### 4.2.3 Score per residue for model 3

- Molecule 1: Nucleoprotein



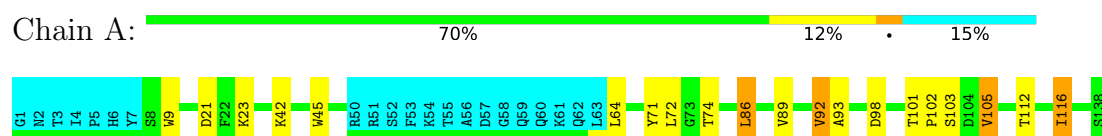
### 4.2.4 Score per residue for model 4

- Molecule 1: Nucleoprotein



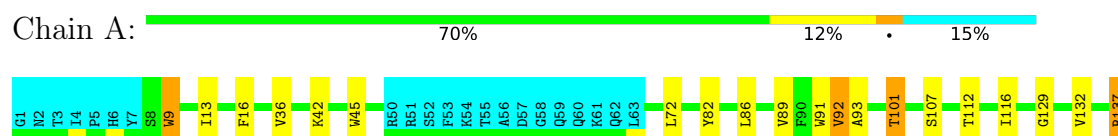
### 4.2.5 Score per residue for model 5

- Molecule 1: Nucleoprotein



### 4.2.6 Score per residue for model 6

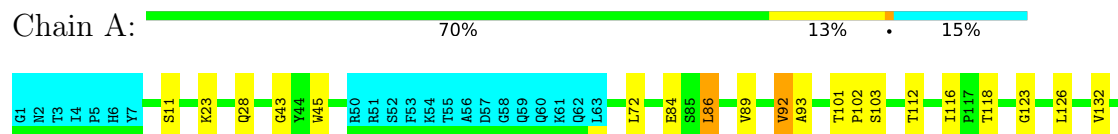
- Molecule 1: Nucleoprotein



S138

#### 4.2.7 Score per residue for model 7

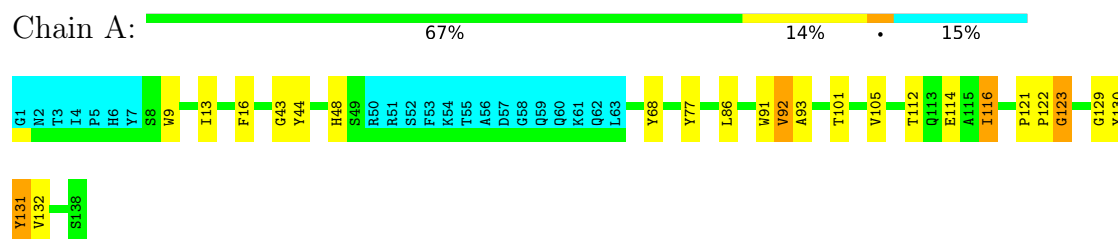
- Molecule 1: Nucleoprotein



S138

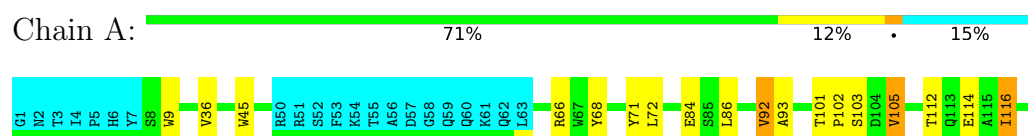
#### 4.2.8 Score per residue for model 8

- Molecule 1: Nucleoprotein

Y131  
V132  
S138

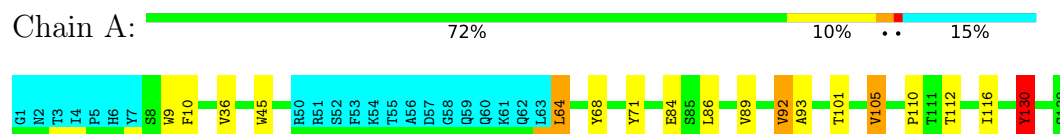
#### 4.2.9 Score per residue for model 9

- Molecule 1: Nucleoprotein



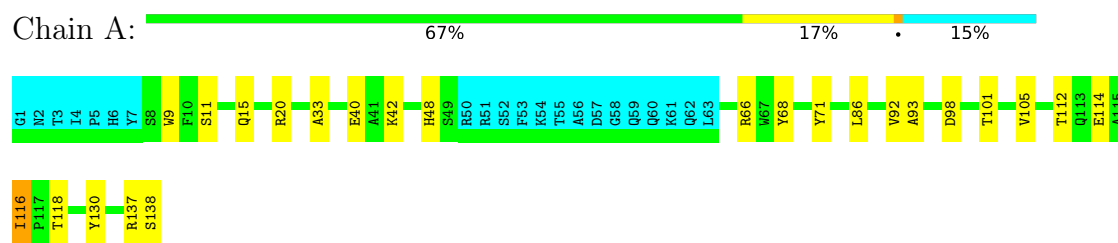
#### 4.2.10 Score per residue for model 10

- Molecule 1: Nucleoprotein



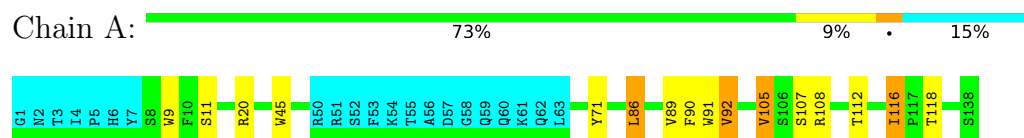
### 4.2.11 Score per residue for model 11

- Molecule 1: Nucleoprotein



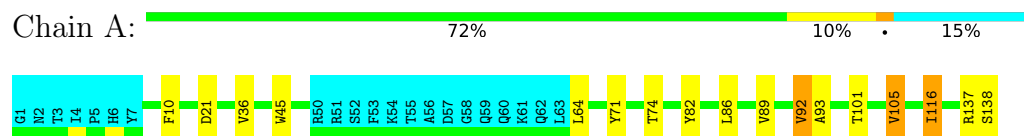
### 4.2.12 Score per residue for model 12

- Molecule 1: Nucleoprotein



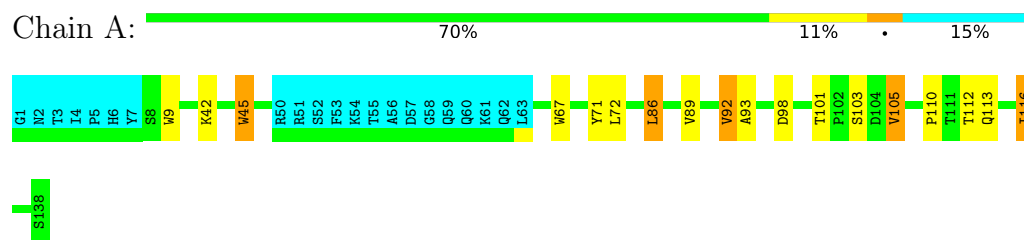
### 4.2.13 Score per residue for model 13

- Molecule 1: Nucleoprotein



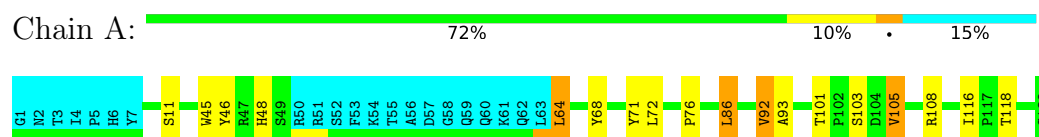
### 4.2.14 Score per residue for model 14

- Molecule 1: Nucleoprotein



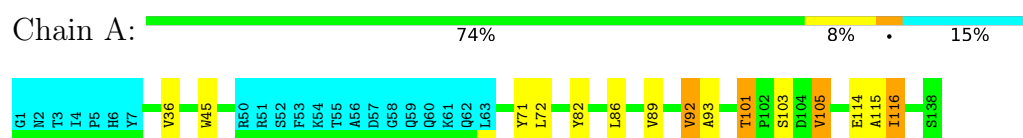
### 4.2.15 Score per residue for model 15

- Molecule 1: Nucleoprotein



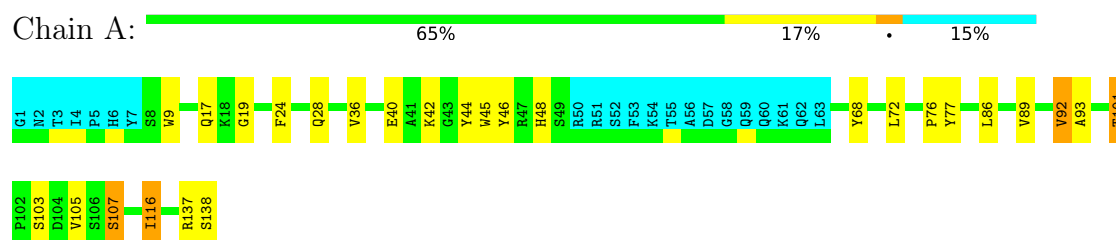
### 4.2.16 Score per residue for model 16

- Molecule 1: Nucleoprotein



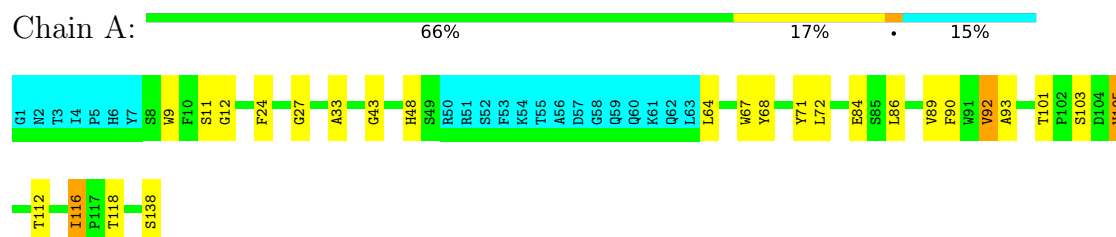
### 4.2.17 Score per residue for model 17

- Molecule 1: Nucleoprotein



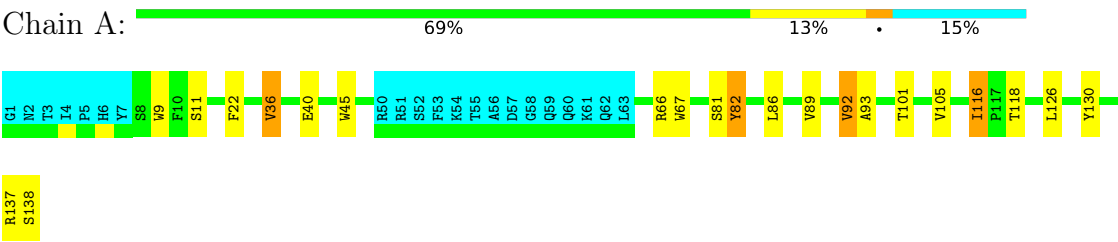
### 4.2.18 Score per residue for model 18

- Molecule 1: Nucleoprotein



4.2.19 Score per residue for model 19

● Molecule 1: Nucleoprotein



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 150000 calculated structures, 19 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | structure calculation |         |
| CS-ROSETTA    | structure calculation |         |
| CS-ROSETTA    | refinement            |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1571           |
| Number of shifts mapped to atoms             | 1571           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 87%            |

## 6 Model quality

### 6.1 Standard geometry

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.54±0.02    | 0±0/966 ( 0.0± 0.0%) | 0.68±0.01   | 0±0/1318 ( 0.0± 0.0%) |
| All | All   | 0.54         | 4/18354 ( 0.0%)      | 0.68        | 1/25042 ( 0.0%)       |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 1.8±0.7   |
| All | All   | 0         | 35        |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 102 | PRO  | N-CD  | -5.27 | 1.40        | 1.47     | 9      | 4     |

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 107 | SER  | CB-CA-C | -5.06 | 109.77      | 115.79   | 17     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group   | Models (Total) |
|-----|-------|-----|------|---------|----------------|
| 1   | A     | 92  | VAL  | Peptide | 17             |
| 1   | A     | 45  | TRP  | Peptide | 6              |
| 1   | A     | 33  | ALA  | Peptide | 3              |

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| Mol | Chain | Res | Type | Group   | Models (Total) |
|-----|-------|-----|------|---------|----------------|
| 1   | A     | 10  | PHE  | Peptide | 3              |
| 1   | A     | 130 | TYR  | Peptide | 3              |
| 1   | A     | 137 | ARG  | Peptide | 1              |
| 1   | A     | 23  | LYS  | Peptide | 1              |
| 1   | A     | 134 | GLY  | Peptide | 1              |

## 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     | 929   | 849      | 851      | 14±3    |
| All | All   | 17651 | 16131    | 16169    | 269     |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:116:ILE:HD12 | 1:A:116:ILE:N    | 0.93     | 1.77        | 13     | 18    |
| 1:A:131:TYR:C    | 1:A:131:TYR:CD1  | 0.77     | 2.60        | 8      | 1     |
| 1:A:116:ILE:N    | 1:A:116:ILE:HD12 | 0.76     | 1.96        | 17     | 1     |
| 1:A:116:ILE:HD12 | 1:A:116:ILE:H    | 0.74     | 1.36        | 13     | 5     |
| 1:A:14:THR:OG1   | 1:A:66:ARG:NH1   | 0.74     | 2.21        | 4      | 1     |
| 1:A:116:ILE:N    | 1:A:116:ILE:CD1  | 0.72     | 2.50        | 13     | 17    |
| 1:A:66:ARG:HD2   | 1:A:138:SER:OXT  | 0.71     | 1.84        | 3      | 2     |
| 1:A:11:SER:HA    | 1:A:138:SER:OXT  | 0.71     | 1.85        | 18     | 1     |
| 1:A:11:SER:O     | 1:A:118:THR:OG1  | 0.68     | 2.11        | 19     | 8     |
| 1:A:66:ARG:NH1   | 1:A:138:SER:O    | 0.68     | 2.26        | 1      | 1     |
| 1:A:116:ILE:H    | 1:A:116:ILE:CD1  | 0.68     | 2.01        | 13     | 2     |
| 1:A:86:LEU:N     | 1:A:86:LEU:HD23  | 0.67     | 2.05        | 5      | 4     |
| 1:A:137:ARG:O    | 1:A:138:SER:CB   | 0.66     | 2.42        | 6      | 1     |
| 1:A:66:ARG:CD    | 1:A:138:SER:OXT  | 0.65     | 2.44        | 3      | 2     |
| 1:A:64:LEU:HD23  | 1:A:64:LEU:N     | 0.64     | 2.06        | 10     | 2     |
| 1:A:86:LEU:N     | 1:A:86:LEU:HD22  | 0.63     | 2.08        | 15     | 14    |
| 1:A:137:ARG:O    | 1:A:138:SER:C    | 0.63     | 2.41        | 11     | 4     |
| 1:A:90:PHE:C     | 1:A:90:PHE:CD2   | 0.60     | 2.79        | 2      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:9:TRP:CE3   | 1:A:9:TRP:N      | 0.59     | 2.68        | 6      | 2     |
| 1:A:72:LEU:O    | 1:A:103:SER:N    | 0.59     | 2.35        | 9      | 10    |
| 1:A:82:TYR:O    | 1:A:82:TYR:CD1   | 0.58     | 2.56        | 19     | 1     |
| 1:A:108:ARG:O   | 1:A:108:ARG:HD2  | 0.57     | 2.00        | 15     | 1     |
| 1:A:45:TRP:CD1  | 1:A:89:VAL:HG13  | 0.55     | 2.37        | 2      | 8     |
| 1:A:137:ARG:O   | 1:A:138:SER:O    | 0.55     | 2.25        | 13     | 5     |
| 1:A:67:TRP:CZ2  | 1:A:130:TYR:CZ   | 0.55     | 2.94        | 1      | 2     |
| 1:A:95:HIS:O    | 1:A:96:GLN:HB2   | 0.55     | 2.03        | 3      | 1     |
| 1:A:40:GLU:OE1  | 1:A:42:LYS:NZ    | 0.54     | 2.33        | 11     | 3     |
| 1:A:64:LEU:HD12 | 1:A:64:LEU:N     | 0.54     | 2.18        | 13     | 2     |
| 1:A:66:ARG:NE   | 1:A:138:SER:OXT  | 0.54     | 2.30        | 19     | 1     |
| 1:A:95:HIS:O    | 1:A:96:GLN:CB    | 0.54     | 2.56        | 3      | 1     |
| 1:A:86:LEU:N    | 1:A:86:LEU:CD2   | 0.53     | 2.71        | 15     | 14    |
| 1:A:108:ARG:O   | 1:A:108:ARG:HD3  | 0.53     | 2.03        | 1      | 1     |
| 1:A:137:ARG:O   | 1:A:138:SER:OG   | 0.53     | 2.22        | 6      | 1     |
| 1:A:86:LEU:HD22 | 1:A:86:LEU:N     | 0.53     | 2.18        | 17     | 1     |
| 1:A:42:LYS:NZ   | 1:A:98:ASP:O     | 0.52     | 2.41        | 5      | 3     |
| 1:A:21:ASP:OD2  | 1:A:23:LYS:NZ    | 0.52     | 2.42        | 5      | 1     |
| 1:A:16:PHE:CZ   | 1:A:131:TYR:CD1  | 0.52     | 2.98        | 8      | 1     |
| 1:A:130:TYR:N   | 1:A:130:TYR:CD1  | 0.52     | 2.77        | 10     | 1     |
| 1:A:17:GLN:HE21 | 1:A:19:GLY:H     | 0.52     | 1.46        | 3      | 2     |
| 1:A:66:ARG:NH2  | 1:A:138:SER:O    | 0.52     | 2.42        | 11     | 1     |
| 1:A:108:ARG:HD2 | 1:A:108:ARG:C    | 0.51     | 2.31        | 15     | 1     |
| 1:A:9:TRP:N     | 1:A:9:TRP:CD2    | 0.50     | 2.79        | 6      | 1     |
| 1:A:44:TYR:OH   | 1:A:77:TYR:O     | 0.49     | 2.30        | 17     | 2     |
| 1:A:8:SER:O     | 1:A:108:ARG:NH1  | 0.49     | 2.46        | 1      | 1     |
| 1:A:134:GLY:O   | 1:A:135:SER:C    | 0.48     | 2.55        | 14     | 1     |
| 1:A:71:TYR:CD2  | 1:A:105:VAL:HG11 | 0.48     | 2.44        | 5      | 13    |
| 1:A:9:TRP:NE1   | 1:A:106:SER:O    | 0.47     | 2.47        | 3      | 1     |
| 1:A:44:TYR:OH   | 1:A:77:TYR:C     | 0.47     | 2.58        | 17     | 1     |
| 1:A:90:PHE:C    | 1:A:90:PHE:HD2   | 0.47     | 2.18        | 2      | 1     |
| 1:A:86:LEU:H    | 1:A:89:VAL:CG1   | 0.47     | 2.22        | 5      | 5     |
| 1:A:92:VAL:O    | 1:A:93:ALA:HB2   | 0.47     | 2.10        | 11     | 18    |
| 1:A:44:TYR:HH   | 1:A:77:TYR:C     | 0.47     | 2.18        | 17     | 1     |
| 1:A:48:HIS:HB2  | 1:A:68:TYR:CE1   | 0.46     | 2.45        | 4      | 7     |
| 1:A:68:TYR:CD1  | 1:A:68:TYR:N     | 0.46     | 2.84        | 11     | 2     |
| 1:A:116:ILE:CD1 | 1:A:116:ILE:H    | 0.46     | 2.22        | 12     | 3     |
| 1:A:16:PHE:N    | 1:A:129:GLY:O    | 0.46     | 2.46        | 6      | 3     |
| 1:A:45:TRP:CD1  | 1:A:89:VAL:CG1   | 0.46     | 2.99        | 12     | 5     |
| 1:A:17:GLN:NE2  | 1:A:18:LYS:O     | 0.45     | 2.49        | 1      | 1     |
| 1:A:72:LEU:CD2  | 1:A:101:THR:O    | 0.45     | 2.65        | 16     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:20:ARG:NE   | 1:A:20:ARG:HA   | 0.45     | 2.26        | 12     | 2     |
| 1:A:43:GLY:O    | 1:A:92:VAL:O    | 0.44     | 2.35        | 7      | 4     |
| 1:A:15:GLN:HB3  | 1:A:130:TYR:CE2 | 0.44     | 2.47        | 11     | 1     |
| 1:A:137:ARG:O   | 1:A:138:SER:HB2 | 0.44     | 2.13        | 6      | 1     |
| 1:A:114:GLU:O   | 1:A:115:ALA:C   | 0.44     | 2.60        | 16     | 1     |
| 1:A:82:TYR:CD2  | 1:A:82:TYR:C    | 0.44     | 2.95        | 4      | 1     |
| 1:A:28:GLN:NE2  | 1:A:123:GLY:O   | 0.44     | 2.50        | 7      | 1     |
| 1:A:36:VAL:CG1  | 1:A:105:VAL:HB  | 0.43     | 2.42        | 4      | 1     |
| 1:A:9:TRP:N     | 1:A:9:TRP:HE3   | 0.43     | 2.11        | 18     | 1     |
| 1:A:45:TRP:CG   | 1:A:89:VAL:HG13 | 0.43     | 2.48        | 5      | 5     |
| 1:A:67:TRP:CZ2  | 1:A:130:TYR:CE2 | 0.43     | 3.06        | 14     | 1     |
| 1:A:22:PHE:CD1  | 1:A:22:PHE:C    | 0.43     | 2.97        | 1      | 2     |
| 1:A:22:PHE:C    | 1:A:22:PHE:CD2  | 0.43     | 2.96        | 2      | 1     |
| 1:A:21:ASP:OD1  | 1:A:21:ASP:C    | 0.43     | 2.62        | 13     | 2     |
| 1:A:91:TRP:CD1  | 1:A:91:TRP:C    | 0.43     | 2.97        | 8      | 1     |
| 1:A:9:TRP:H     | 1:A:9:TRP:HE3   | 0.43     | 1.45        | 6      | 1     |
| 1:A:131:TYR:CD1 | 1:A:131:TYR:O   | 0.43     | 2.71        | 8      | 1     |
| 1:A:121:PRO:O   | 1:A:123:GLY:N   | 0.42     | 2.52        | 8      | 1     |
| 1:A:107:SER:O   | 1:A:108:ARG:C   | 0.42     | 2.62        | 12     | 1     |
| 1:A:98:ASP:OD1  | 1:A:98:ASP:C    | 0.42     | 2.63        | 3      | 1     |
| 1:A:91:TRP:CD1  | 1:A:92:VAL:N    | 0.42     | 2.88        | 12     | 2     |
| 1:A:10:PHE:CZ   | 1:A:31:PRO:CG   | 0.42     | 3.03        | 3      | 1     |
| 1:A:36:VAL:CG2  | 1:A:40:GLU:HB2  | 0.42     | 2.44        | 19     | 2     |
| 1:A:48:HIS:CB   | 1:A:68:TYR:CE1  | 0.42     | 3.03        | 17     | 1     |
| 1:A:12:GLY:CA   | 1:A:67:TRP:O    | 0.42     | 2.68        | 18     | 1     |
| 1:A:131:TYR:O   | 1:A:131:TYR:HD1 | 0.42     | 1.98        | 8      | 1     |
| 1:A:66:ARG:NE   | 1:A:68:TYR:OH   | 0.42     | 2.52        | 9      | 1     |
| 1:A:81:SER:O    | 1:A:82:TYR:C    | 0.42     | 2.63        | 19     | 1     |
| 1:A:9:TRP:CD1   | 1:A:107:SER:HG  | 0.42     | 2.33        | 17     | 1     |
| 1:A:131:TYR:C   | 1:A:131:TYR:HD1 | 0.41     | 2.15        | 8      | 1     |
| 1:A:24:PHE:CD1  | 1:A:28:GLN:O    | 0.41     | 2.74        | 17     | 1     |
| 1:A:90:PHE:CD2  | 1:A:91:TRP:O    | 0.41     | 2.73        | 12     | 1     |
| 1:A:24:PHE:CZ   | 1:A:90:PHE:CD2  | 0.41     | 3.09        | 1      | 1     |
| 1:A:110:PRO:HA  | 1:A:113:GLN:O   | 0.40     | 2.16        | 14     | 1     |
| 1:A:46:TYR:CZ   | 1:A:76:PRO:HG2  | 0.40     | 2.52        | 17     | 3     |
| 1:A:89:VAL:CG1  | 1:A:90:PHE:N    | 0.40     | 2.84        | 18     | 1     |
| 1:A:27:GLY:HA2  | 1:A:93:ALA:O    | 0.40     | 2.17        | 18     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|------------|-------------|----|
| 1   | A     | 116/138 (84%)   | 109±2 (94±1%) | 7±2 (6±1%) | 1±1 (0±1%) | 26          | 74 |
| All | All   | 2204/2622 (84%) | 2070 (94%)    | 124 (6%)   | 10 (0%)    | 26          | 74 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 84  | GLU  | 5              |
| 1   | A     | 105 | VAL  | 1              |
| 1   | A     | 107 | SER  | 1              |
| 1   | A     | 122 | PRO  | 1              |
| 1   | A     | 123 | GLY  | 1              |
| 1   | A     | 82  | TYR  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 96/114 (84%)    | 90±1 (94±1%) | 6±1 (6±1%) | 19          | 69 |
| All | All   | 1824/2166 (84%) | 1716 (94%)   | 108 (6%)   | 19          | 69 |

All 18 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     | 101 | THR  | 17             |
| 1   | A     | 105 | VAL  | 15             |
| 1   | A     | 112 | THR  | 13             |
| 1   | A     | 116 | ILE  | 13             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 36  | VAL  | 11             |
| 1   | A     | 9   | TRP  | 11             |
| 1   | A     | 86  | LEU  | 5              |
| 1   | A     | 114 | GLU  | 3              |
| 1   | A     | 64  | LEU  | 3              |
| 1   | A     | 82  | TYR  | 3              |
| 1   | A     | 132 | VAL  | 3              |
| 1   | A     | 42  | LYS  | 2              |
| 1   | A     | 74  | THR  | 2              |
| 1   | A     | 13  | ILE  | 2              |
| 1   | A     | 126 | LEU  | 2              |
| 1   | A     | 131 | TYR  | 1              |
| 1   | A     | 130 | TYR  | 1              |
| 1   | A     | 24  | PHE  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

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

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1571 |
| Number of shifts mapped to atoms        | 1571 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 13   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 138      | $0.18 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 122      | $0.12 \pm 0.07$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 117      | $0.34 \pm 0.14$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 120      | $-1.23 \pm 0.39$                | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1325 atoms were assigned a chemical shift out of a possible 1521. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 550/577 (95%) | 232/237 (98%) | 217/234 (93%)   | 101/106 (95%)   |
| Sidechain | 635/723 (88%) | 430/469 (92%) | 197/225 (88%)   | 8/29 (28%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 140/221 (63%)   | 73/108 (68%)   | 63/109 (58%)    | 4/4 (100%)      |
| Overall  | 1325/1521 (87%) | 735/814 (90%)  | 477/568 (84%)   | 113/139 (81%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1571 atoms were assigned a chemical shift out of a possible 1817. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 649/682 (95%)   | 274/280 (98%)  | 255/276 (92%)   | 120/126 (95%)   |
| Sidechain | 773/889 (87%)   | 523/574 (91%)  | 239/274 (87%)   | 11/41 (27%)     |
| Aromatic  | 149/246 (61%)   | 78/121 (64%)   | 67/121 (55%)    | 4/4 (100%)      |
| Overall   | 1571/1817 (86%) | 875/975 (90%)  | 561/671 (84%)   | 135/171 (79%)   |

#### 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.

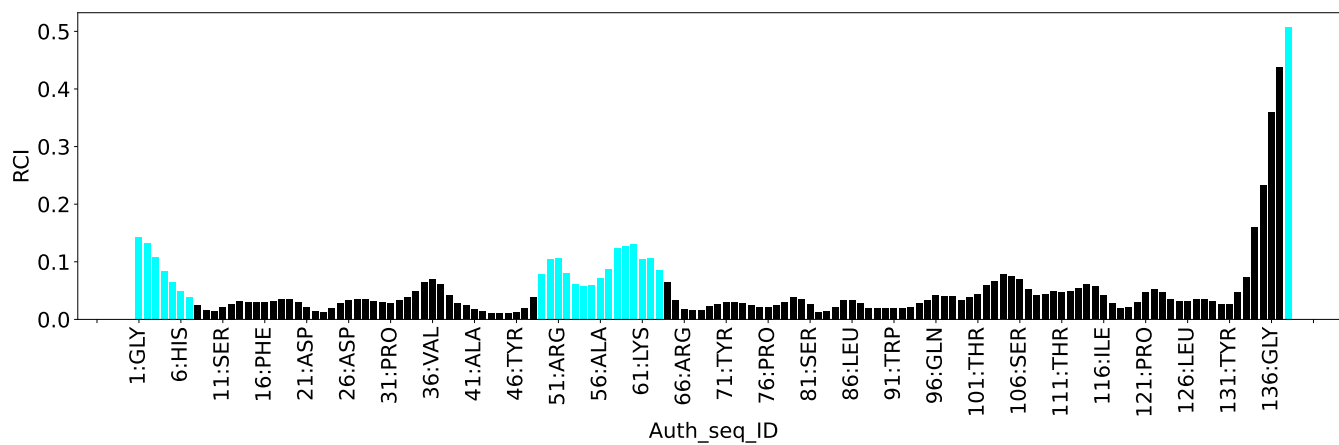
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 47  | ARG  | HD2  | 0.10       | 1.97 – 4.26         | -13.2   |
| 1       | A     | 47  | ARG  | HB2  | -1.36      | 0.52 – 3.08         | -12.3   |
| 1       | A     | 47  | ARG  | HB3  | -1.35      | 0.43 – 3.11         | -11.6   |
| 1       | A     | 47  | ARG  | HD3  | 0.10       | 1.81 – 4.39         | -11.6   |
| 1       | A     | 108 | ARG  | HB3  | -0.84      | 0.43 – 3.11         | -9.7    |
| 1       | A     | 83  | GLY  | H    | 3.04       | 5.23 – 11.42        | -8.5    |
| 1       | A     | 29  | GLY  | HA2  | 1.47       | 2.15 – 5.77         | -6.9    |
| 1       | A     | 31  | PRO  | HD3  | 1.15       | 1.76 – 5.48         | -6.6    |
| 1       | A     | 127 | PRO  | HG3  | -0.09      | 0.33 – 3.48         | -6.3    |
| 1       | A     | 31  | PRO  | HG2  | 0.13       | 0.41 – 3.45         | -5.9    |
| 1       | A     | 31  | PRO  | HB3  | 0.12       | 0.25 – 3.76         | -5.4    |
| 1       | A     | 82  | TYR  | HA   | 1.78       | 1.87 – 7.33         | -5.2    |
| 1       | A     | 76  | PRO  | HD3  | 1.74       | 1.76 – 5.48         | -5.0    |

#### 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                                | 2568  |
| Intra-residue ( $ i-j =0$ )                              | 0     |
| Sequential ( $ i-j =1$ )                                 | 1221  |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 444   |
| Long range ( $ i-j \geq 5$ )                             | 903   |
| 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                         | 18.6  |
| Number of long range restraints per residue <sup>1</sup> | 6.5   |

<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)  | 43.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 72.7                                   | 0.5     |
| >0.5 (Large)     | 234.8                                  | 6.55    |

### 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 ⓘ

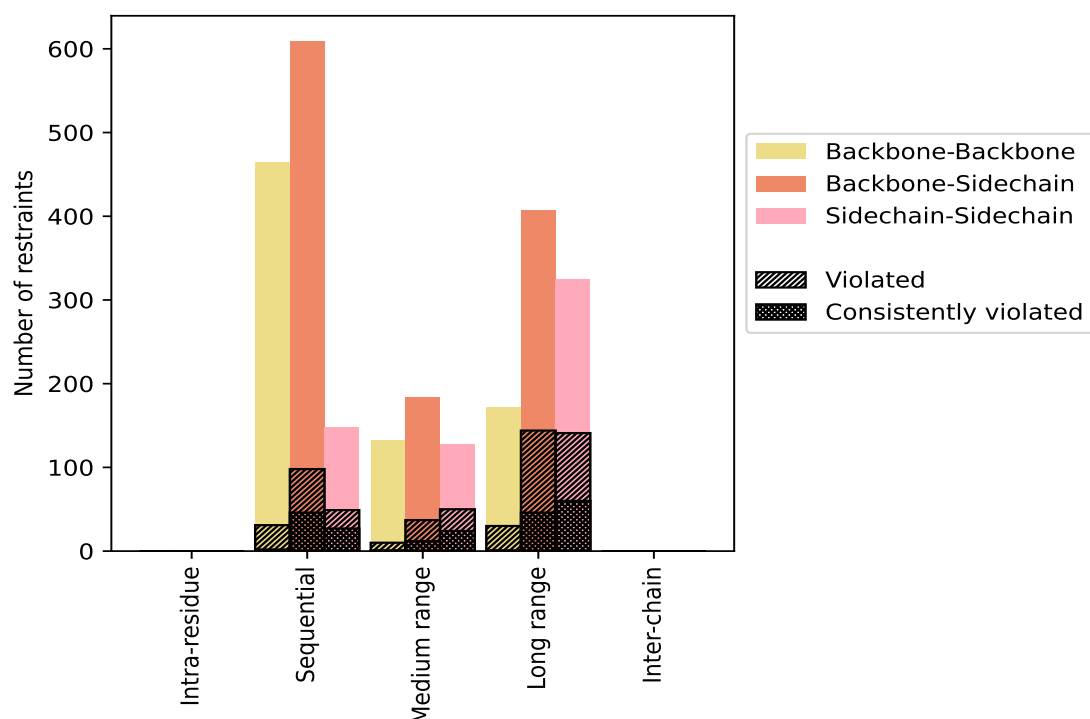
### 9.1 Summary of distance violations ⓘ

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> |
| Intra-residue ( $ i-j =0$ )            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| 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            |
| Sequential ( $ i-j =1$ )               | 1221  | 47.5           | 178                   | 14.6           | 6.9            | 75                                 | 6.1            | 2.9            |
| Backbone-Backbone                      | 464   | 18.1           | 31                    | 6.7            | 1.2            | 2                                  | 0.4            | 0.1            |
| Backbone-Sidechain                     | 609   | 23.7           | 98                    | 16.1           | 3.8            | 46                                 | 7.6            | 1.8            |
| Sidechain-Sidechain                    | 148   | 5.8            | 49                    | 33.1           | 1.9            | 27                                 | 18.2           | 1.1            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 444   | 17.3           | 97                    | 21.8           | 3.8            | 37                                 | 8.3            | 1.4            |
| Backbone-Backbone                      | 132   | 5.1            | 10                    | 7.6            | 0.4            | 1                                  | 0.8            | 0.0            |
| Backbone-Sidechain                     | 184   | 7.2            | 37                    | 20.1           | 1.4            | 12                                 | 6.5            | 0.5            |
| Sidechain-Sidechain                    | 128   | 5.0            | 50                    | 39.1           | 1.9            | 24                                 | 18.8           | 0.9            |
| Long range ( $ i-j \geq 5$ )           | 903   | 35.2           | 315                   | 34.9           | 12.3           | 107                                | 11.8           | 4.2            |
| Backbone-Backbone                      | 172   | 6.7            | 30                    | 17.4           | 1.2            | 1                                  | 0.6            | 0.0            |
| Backbone-Sidechain                     | 407   | 15.8           | 144                   | 35.4           | 5.6            | 46                                 | 11.3           | 1.8            |
| Sidechain-Sidechain                    | 324   | 12.6           | 141                   | 43.5           | 5.5            | 60                                 | 18.5           | 2.3            |
| Inter-chain                            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| 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            |
| Hydrogen bond                          | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Disulfide bond                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 2568  | 100.0          | 590                   | 23.0           | 23.0           | 219                                | 8.5            | 8.5            |
| Backbone-Backbone                      | 768   | 29.9           | 71                    | 9.2            | 2.8            | 4                                  | 0.5            | 0.2            |
| Backbone-Sidechain                     | 1200  | 46.7           | 279                   | 23.2           | 10.9           | 104                                | 8.7            | 4.0            |
| Sidechain-Sidechain                    | 600   | 23.4           | 240                   | 40.0           | 9.3            | 111                                | 18.5           | 4.3            |

<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        | 0                    | 107             | 63              | 176             | 0               | 346   | 0.97     | 4.74    | 0.83                | 0.74       |
| 2        | 0                    | 111             | 60              | 188             | 0               | 359   | 0.99     | 6.17    | 0.83                | 0.82       |
| 3        | 0                    | 116             | 58              | 178             | 0               | 352   | 1.0      | 6.12    | 0.84                | 0.76       |
| 4        | 0                    | 117             | 55              | 181             | 0               | 353   | 1.0      | 5.65    | 0.86                | 0.75       |
| 5        | 0                    | 110             | 55              | 186             | 0               | 351   | 1.02     | 6.48    | 0.85                | 0.85       |
| 6        | 0                    | 109             | 50              | 191             | 0               | 350   | 0.97     | 6.11    | 0.84                | 0.77       |
| 7        | 0                    | 114             | 54              | 186             | 0               | 354   | 0.96     | 5.96    | 0.83                | 0.74       |
| 8        | 0                    | 109             | 62              | 192             | 0               | 363   | 0.95     | 5.22    | 0.84                | 0.7        |
| 9        | 0                    | 112             | 60              | 189             | 0               | 361   | 0.99     | 6.13    | 0.83                | 0.77       |
| 10       | 0                    | 106             | 61              | 196             | 0               | 363   | 0.97     | 6.08    | 0.85                | 0.76       |

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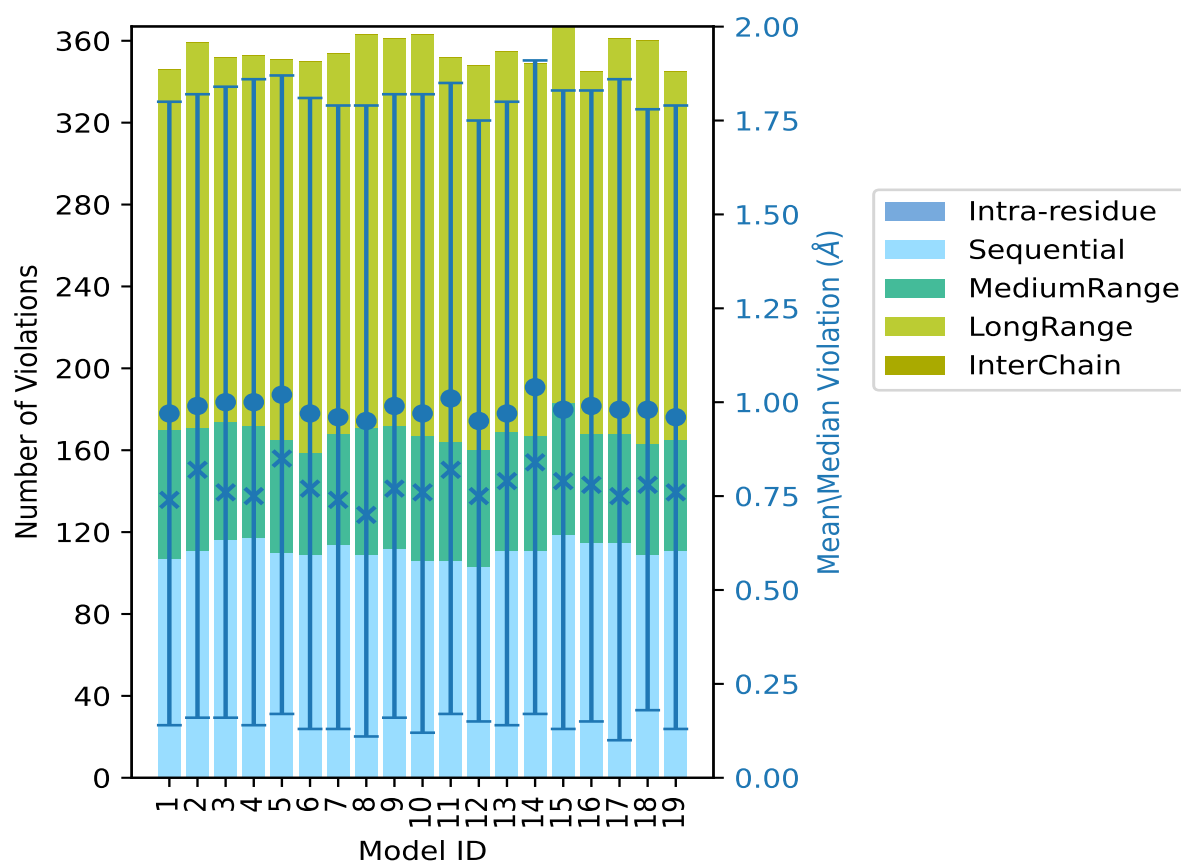
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 106             | 58              | 188             | 0               | 352   | 1.01     | 4.71    | 0.84                | 0.82       |
| 12       | 0                    | 103             | 57              | 188             | 0               | 348   | 0.95     | 4.73    | 0.8                 | 0.75       |
| 13       | 0                    | 111             | 58              | 186             | 0               | 355   | 0.97     | 6.21    | 0.83                | 0.79       |
| 14       | 0                    | 111             | 56              | 182             | 0               | 349   | 1.04     | 6.55    | 0.87                | 0.84       |
| 15       | 0                    | 119             | 64              | 184             | 0               | 367   | 0.98     | 5.88    | 0.85                | 0.79       |
| 16       | 0                    | 115             | 53              | 177             | 0               | 345   | 0.99     | 5.51    | 0.84                | 0.78       |
| 17       | 0                    | 115             | 53              | 193             | 0               | 361   | 0.98     | 5.93    | 0.88                | 0.75       |
| 18       | 0                    | 109             | 54              | 197             | 0               | 360   | 0.98     | 4.61    | 0.8                 | 0.78       |
| 19       | 0                    | 111             | 54              | 180             | 0               | 345   | 0.96     | 5.7     | 0.83                | 0.76       |

<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

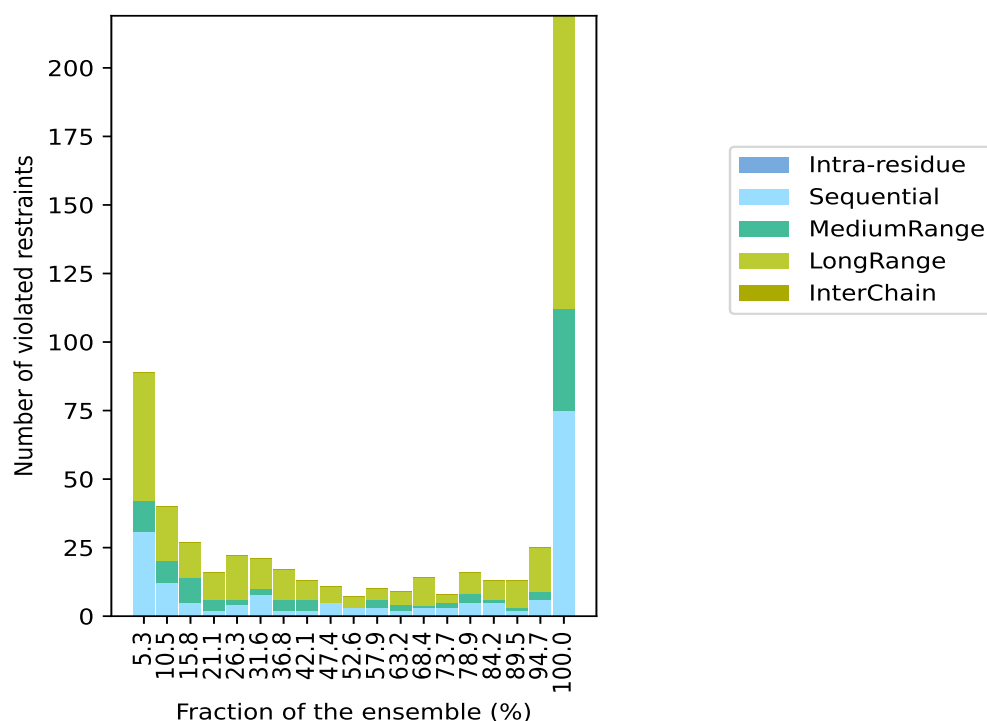
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1978(IR:0, SQ:1043, MR:347, LR:588, IC:0) restraints are 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>       | %     |
| 0                             | 31              | 11              | 47              | 0               | 89    | 1                        | 5.3   |
| 0                             | 12              | 8               | 20              | 0               | 40    | 2                        | 10.5  |
| 0                             | 5               | 9               | 13              | 0               | 27    | 3                        | 15.8  |
| 0                             | 2               | 4               | 10              | 0               | 16    | 4                        | 21.1  |
| 0                             | 4               | 2               | 16              | 0               | 22    | 5                        | 26.3  |
| 0                             | 8               | 2               | 11              | 0               | 21    | 6                        | 31.6  |
| 0                             | 2               | 4               | 11              | 0               | 17    | 7                        | 36.8  |
| 0                             | 2               | 4               | 7               | 0               | 13    | 8                        | 42.1  |
| 0                             | 5               | 0               | 6               | 0               | 11    | 9                        | 47.4  |
| 0                             | 3               | 0               | 4               | 0               | 7     | 10                       | 52.6  |
| 0                             | 3               | 3               | 4               | 0               | 10    | 11                       | 57.9  |
| 0                             | 2               | 2               | 5               | 0               | 9     | 12                       | 63.2  |
| 0                             | 3               | 1               | 10              | 0               | 14    | 13                       | 68.4  |
| 0                             | 3               | 2               | 3               | 0               | 8     | 14                       | 73.7  |
| 0                             | 5               | 3               | 8               | 0               | 16    | 15                       | 78.9  |
| 0                             | 5               | 1               | 7               | 0               | 13    | 16                       | 84.2  |
| 0                             | 2               | 1               | 10              | 0               | 13    | 17                       | 89.5  |
| 0                             | 6               | 3               | 16              | 0               | 25    | 18                       | 94.7  |
| 0                             | 75              | 37              | 107             | 0               | 219   | 19                       | 100.0 |

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

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

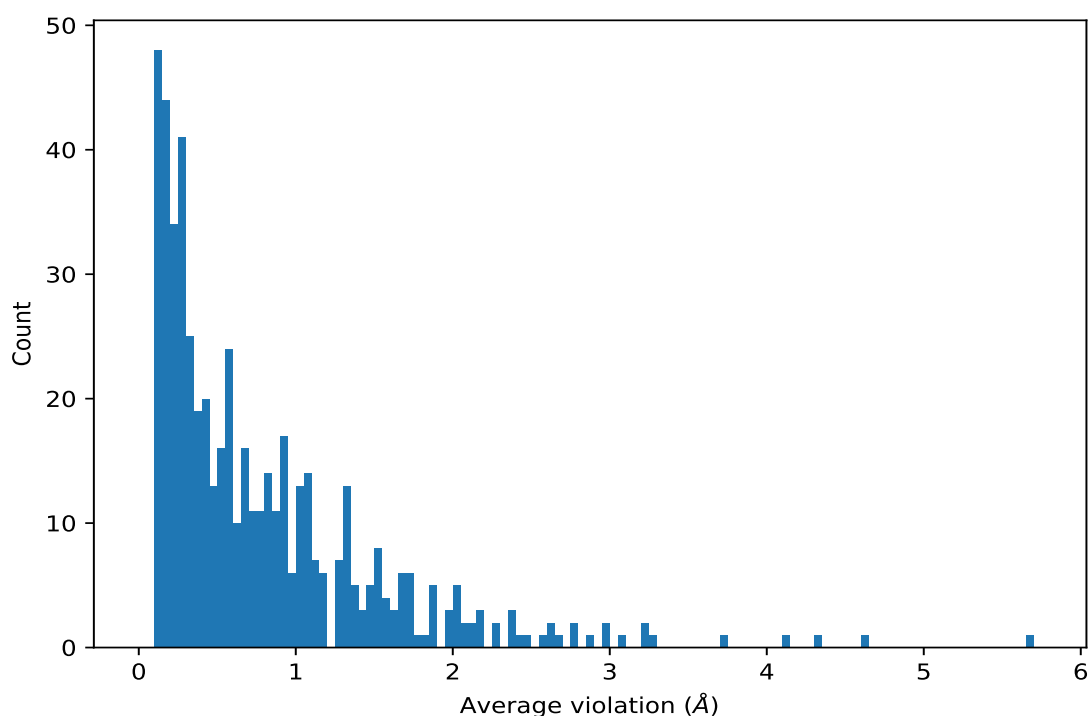
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 19                  | 5.68     | 0.65                | 5.93       |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 19                  | 4.63     | 0.1                 | 4.62       |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 19                  | 4.34     | 0.1                 | 4.33       |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 19                  | 4.12     | 0.1                 | 4.11       |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 19                  | 3.73     | 0.18                | 3.71       |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 19                  | 3.27     | 1.05                | 3.64       |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 19                  | 3.21     | 1.0                 | 3.3        |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 19                  | 3.2      | 0.14                | 3.24       |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 19                  | 3.06     | 0.09                | 3.06       |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 19                  | 2.98     | 0.14                | 3.02       |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 19                  | 2.97     | 0.12                | 2.99       |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB | 19                  | 2.86     | 0.09                | 2.87       |
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB  | 19                  | 2.76     | 0.17                | 2.7        |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB  | 19                  | 2.76     | 0.17                | 2.7        |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB  | 19                  | 2.68     | 0.33                | 2.58       |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB  | 19                  | 2.63     | 0.34                | 2.53       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,260)  | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 19                  | 2.58     | 0.09                | 2.6        |
| (2,42)   | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 19                  | 2.48     | 0.14                | 2.51       |
| (2,171)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 19                  | 2.43     | 0.2                 | 2.44       |
| (2,514)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 19                  | 2.4      | 0.52                | 2.51       |
| (2,800)  | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 19                  | 2.35     | 0.09                | 2.37       |
| (2,829)  | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 19                  | 2.35     | 0.75                | 2.26       |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 19                  | 2.3      | 0.09                | 2.3        |
| (2,935)  | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 19                  | 2.28     | 0.09                | 2.26       |
| (1,308)  | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 19                  | 2.18     | 0.12                | 2.2        |
| (2,833)  | 1:13:A:ILE:CB   | 1:120:A:PHE:CB  | 19                  | 2.15     | 0.2                 | 2.09       |
| (2,818)  | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 19                  | 2.15     | 0.2                 | 2.09       |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 19                  | 2.11     | 0.41                | 2.14       |
| (2,437)  | 1:84:A:GLU:H    | 1:86:A:LEU:CB   | 19                  | 2.07     | 0.18                | 2.03       |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 19                  | 2.06     | 0.39                | 2.22       |
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 19                  | 2.04     | 0.2                 | 2.05       |
| (2,558)  | 1:84:A:GLU:CB   | 1:86:A:LEU:CB   | 19                  | 2.03     | 0.13                | 2.0        |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 19                  | 2.03     | 0.27                | 1.92       |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 19                  | 2.03     | 0.27                | 1.92       |
| (2,866)  | 1:41:A:ALA:CB   | 1:71:A:TYR:CB   | 19                  | 2.01     | 0.14                | 2.0        |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 19                  | 1.96     | 0.2                 | 1.97       |
| (2,520)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 19                  | 1.96     | 0.12                | 1.94       |
| (2,626)  | 1:99:A:THR:CB   | 1:42:A:LYS:CB   | 19                  | 1.9      | 0.11                | 1.93       |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 19                  | 1.88     | 0.2                 | 1.89       |
| (2,423)  | 1:14:A:THR:H    | 1:126:A:LEU:CB  | 19                  | 1.87     | 0.21                | 1.95       |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 19                  | 1.85     | 0.21                | 1.78       |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB  | 19                  | 1.84     | 0.06                | 1.83       |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 19                  | 1.79     | 0.1                 | 1.83       |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 19                  | 1.74     | 0.1                 | 1.78       |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 19                  | 1.74     | 0.21                | 1.8        |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 19                  | 1.73     | 0.07                | 1.72       |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 19                  | 1.72     | 0.39                | 1.75       |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 19                  | 1.72     | 0.3                 | 1.8        |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 19                  | 1.71     | 0.19                | 1.77       |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 19                  | 1.7      | 0.1                 | 1.68       |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 19                  | 1.68     | 0.28                | 1.75       |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 19                  | 1.67     | 0.35                | 1.73       |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 19                  | 1.66     | 0.07                | 1.69       |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 19                  | 1.66     | 0.17                | 1.7        |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 19                  | 1.64     | 0.22                | 1.53       |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 19                  | 1.62     | 0.48                | 1.6        |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 19                  | 1.59     | 0.02                | 1.59       |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 19                  | 1.58     | 0.09                | 1.61       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 19                  | 1.56     | 0.06                | 1.53       |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 19                  | 1.55     | 0.32                | 1.49       |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 19                  | 1.52     | 0.11                | 1.51       |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 19                  | 1.52     | 0.35                | 1.58       |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 19                  | 1.52     | 0.13                | 1.5        |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 19                  | 1.52     | 0.13                | 1.5        |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 19                  | 1.51     | 0.78                | 1.43       |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 19                  | 1.51     | 0.09                | 1.47       |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 19                  | 1.49     | 0.14                | 1.47       |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 19                  | 1.48     | 0.19                | 1.54       |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 19                  | 1.47     | 0.36                | 1.51       |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 19                  | 1.46     | 0.26                | 1.46       |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 19                  | 1.46     | 0.35                | 1.35       |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 19                  | 1.44     | 0.14                | 1.47       |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 19                  | 1.43     | 0.39                | 1.43       |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 19                  | 1.41     | 0.22                | 1.36       |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 19                  | 1.36     | 0.13                | 1.38       |
| (2,905)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 19                  | 1.35     | 0.01                | 1.35       |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 19                  | 1.35     | 0.4                 | 1.44       |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 19                  | 1.33     | 0.01                | 1.33       |
| (2,442)  | 1:37:A:PRO:CB   | 1:36:A:VAL:CB   | 19                  | 1.33     | 0.11                | 1.37       |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 19                  | 1.32     | 0.35                | 1.38       |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 19                  | 1.31     | 0.01                | 1.31       |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 19                  | 1.31     | 0.01                | 1.31       |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 19                  | 1.31     | 0.18                | 1.35       |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 19                  | 1.31     | 0.18                | 1.35       |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 19                  | 1.3      | 0.32                | 1.19       |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 19                  | 1.3      | 0.27                | 1.19       |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 19                  | 1.29     | 0.53                | 1.55       |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 19                  | 1.29     | 0.27                | 1.19       |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 19                  | 1.29     | 0.09                | 1.3        |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 19                  | 1.29     | 0.09                | 1.3        |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 19                  | 1.29     | 0.45                | 1.46       |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 19                  | 1.29     | 0.45                | 1.46       |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 19                  | 1.26     | 0.52                | 1.37       |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 19                  | 1.2      | 0.4                 | 1.32       |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 19                  | 1.19     | 0.1                 | 1.2        |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 19                  | 1.18     | 0.04                | 1.19       |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 19                  | 1.16     | 0.15                | 1.18       |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 19                  | 1.16     | 0.62                | 0.9        |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 19                  | 1.15     | 0.01                | 1.15       |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 19                  | 1.14     | 0.22                | 1.09       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 19                  | 1.13     | 0.01                | 1.13       |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 19                  | 1.12     | 0.2                 | 1.18       |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 19                  | 1.11     | 0.09                | 1.08       |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 19                  | 1.11     | 0.09                | 1.08       |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 19                  | 1.1      | 0.15                | 1.1        |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 19                  | 1.09     | 0.05                | 1.1        |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 19                  | 1.08     | 0.01                | 1.08       |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 19                  | 1.07     | 0.16                | 1.06       |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 19                  | 1.06     | 0.11                | 1.08       |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 19                  | 1.06     | 0.11                | 1.08       |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 19                  | 1.06     | 0.04                | 1.06       |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 19                  | 1.05     | 0.12                | 1.03       |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 19                  | 1.05     | 0.27                | 0.93       |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 19                  | 1.05     | 0.27                | 0.93       |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 19                  | 1.05     | 0.27                | 0.93       |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 19                  | 1.05     | 0.03                | 1.05       |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 19                  | 1.03     | 0.32                | 0.98       |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 19                  | 1.02     | 0.05                | 1.02       |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 19                  | 1.02     | 0.22                | 0.98       |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 19                  | 1.01     | 0.07                | 1.01       |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 19                  | 1.01     | 0.07                | 1.01       |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 19                  | 1.0      | 0.08                | 0.99       |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 19                  | 1.0      | 0.25                | 0.91       |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 19                  | 0.98     | 0.21                | 0.9        |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 19                  | 0.98     | 0.11                | 1.04       |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 19                  | 0.98     | 0.1                 | 0.97       |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 19                  | 0.97     | 0.31                | 0.9        |
| (2,198)  | 1:126:A:LEU:CA  | 1:127:A:PRO:CB  | 19                  | 0.96     | 0.01                | 0.96       |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB   | 19                  | 0.95     | 0.09                | 0.97       |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 19                  | 0.94     | 0.41                | 1.04       |
| (2,901)  | 1:37:A:PRO:CA   | 1:38:A:PRO:CB   | 19                  | 0.94     | 0.01                | 0.94       |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 19                  | 0.94     | 0.21                | 0.85       |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 19                  | 0.93     | 0.01                | 0.94       |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 19                  | 0.93     | 0.01                | 0.94       |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 19                  | 0.93     | 0.03                | 0.95       |
| (2,208)  | 1:126:A:LEU:CA  | 1:127:A:PRO:CB  | 19                  | 0.92     | 0.01                | 0.92       |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 19                  | 0.92     | 0.43                | 0.82       |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 19                  | 0.91     | 0.17                | 0.93       |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 19                  | 0.91     | 0.31                | 0.9        |
| (2,776)  | 1:28:A:GLN:H    | 1:30:A:VAL:CB   | 19                  | 0.9      | 0.11                | 0.93       |
| (2,900)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 19                  | 0.9      | 0.02                | 0.91       |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3  | 19                  | 0.89     | 0.19                | 0.88       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,1086) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB   | 19                  | 0.89     | 0.35                | 0.78       |
| (2,899)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA  | 19                  | 0.88     | 0.01                | 0.88       |
| (2,1146) | 1:101:A:THR:CA | 1:102:A:PRO:CB  | 19                  | 0.87     | 0.02                | 0.88       |
| (2,1123) | 1:126:A:LEU:CB | 1:13:A:ILE:CB   | 19                  | 0.87     | 0.09                | 0.88       |
| (2,1153) | 1:93:A:ALA:H   | 1:30:A:VAL:CB   | 19                  | 0.85     | 0.08                | 0.86       |
| (1,310)  | 1:46:A:TYR:HB2 | 1:68:A:TYR:HB2  | 19                  | 0.85     | 0.22                | 0.78       |
| (2,860)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 19                  | 0.82     | 0.35                | 0.8        |
| (2,886)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 19                  | 0.82     | 0.35                | 0.8        |
| (2,84)   | 1:44:A:TYR:CB  | 1:91:A:TRP:CB   | 19                  | 0.82     | 0.23                | 0.89       |
| (2,797)  | 1:126:A:LEU:CB | 1:127:A:PRO:CB  | 19                  | 0.82     | 0.07                | 0.84       |
| (2,1147) | 1:101:A:THR:CB | 1:102:A:PRO:CB  | 19                  | 0.82     | 0.14                | 0.75       |
| (2,727)  | 1:114:A:GLU:CB | 1:116:A:ILE:CB  | 19                  | 0.81     | 0.22                | 0.87       |
| (1,1278) | 1:78:A:ALA:HA  | 1:76:A:PRO:HD3  | 19                  | 0.8      | 0.08                | 0.78       |
| (2,898)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB    | 19                  | 0.79     | 0.05                | 0.79       |
| (2,426)  | 1:40:A:GLU:H   | 1:36:A:VAL:CB   | 19                  | 0.77     | 0.25                | 0.89       |
| (2,587)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB   | 19                  | 0.77     | 0.17                | 0.83       |
| (2,109)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CB    | 19                  | 0.77     | 0.05                | 0.77       |
| (2,670)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA  | 19                  | 0.77     | 0.01                | 0.77       |
| (2,105)  | 1:24:A:PHE:CA  | 1:125:A:ILE:CB  | 19                  | 0.76     | 0.24                | 0.74       |
| (2,762)  | 1:126:A:LEU:H  | 1:127:A:PRO:CB  | 19                  | 0.75     | 0.23                | 0.7        |
| (1,270)  | 1:112:A:THR:H  | 1:109:A:ASP:HB2 | 19                  | 0.74     | 0.12                | 0.76       |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2  | 19                  | 0.73     | 0.61                | 0.59       |
| (1,851)  | 1:28:A:GLN:H   | 1:25:A:SER:HB3  | 19                  | 0.73     | 0.17                | 0.73       |
| (2,366)  | 1:120:A:PHE:CB | 1:31:A:PRO:CB   | 19                  | 0.72     | 0.24                | 0.61       |
| (2,192)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 19                  | 0.71     | 0.01                | 0.71       |
| (1,789)  | 1:83:A:GLY:HA2 | 1:84:A:GLU:HG2  | 19                  | 0.71     | 0.13                | 0.73       |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 19                  | 0.7      | 0.06                | 0.69       |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 19                  | 0.7      | 0.13                | 0.66       |
| (1,780)  | 1:131:A:TYR:H  | 1:16:A:PHE:HB3  | 19                  | 0.66     | 0.17                | 0.71       |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 19                  | 0.65     | 0.08                | 0.64       |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 19                  | 0.65     | 0.08                | 0.66       |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12 | 19                  | 0.65     | 0.07                | 0.65       |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 19                  | 0.64     | 0.01                | 0.64       |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2  | 19                  | 0.63     | 0.16                | 0.61       |
| (1,840)  | 1:120:A:PHE:HA | 1:32:A:ILE:HG12 | 19                  | 0.62     | 0.23                | 0.71       |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 19                  | 0.61     | 0.01                | 0.61       |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 19                  | 0.61     | 0.01                | 0.61       |
| (2,9)    | 1:4:A:ILE:CB   | 1:6:A:HIS:CB    | 19                  | 0.61     | 0.33                | 0.58       |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB  | 19                  | 0.6      | 0.15                | 0.64       |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB   | 19                  | 0.6      | 0.17                | 0.66       |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2  | 19                  | 0.6      | 0.12                | 0.6        |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA  | 19                  | 0.6      | 0.01                | 0.6        |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB    | 19                  | 0.6      | 0.05                | 0.6        |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB   | 19                  | 0.6      | 0.09                | 0.61       |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 19                  | 0.59     | 0.04                | 0.6        |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 19                  | 0.59     | 0.01                | 0.59       |
| (1,1334) | 1:16:A:PHE:HB3 | 1:130:A:TYR:HB3 | 19                  | 0.58     | 0.26                | 0.53       |
| (1,380)  | 1:31:A:PRO:HA  | 1:32:A:ILE:HG12 | 19                  | 0.58     | 0.2                 | 0.55       |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB  | 19                  | 0.57     | 0.04                | 0.57       |
| (2,1102) | 1:130:A:TYR:H  | 1:17:A:GLN:CB   | 19                  | 0.56     | 0.2                 | 0.58       |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB   | 19                  | 0.56     | 0.09                | 0.54       |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB   | 19                  | 0.56     | 0.06                | 0.57       |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 19                  | 0.55     | 0.06                | 0.52       |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 19                  | 0.54     | 0.07                | 0.55       |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB  | 19                  | 0.53     | 0.06                | 0.56       |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB   | 19                  | 0.53     | 0.04                | 0.54       |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB   | 19                  | 0.52     | 0.08                | 0.52       |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB   | 19                  | 0.51     | 0.13                | 0.56       |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB  | 19                  | 0.5      | 0.07                | 0.53       |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2  | 19                  | 0.49     | 0.16                | 0.52       |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB   | 19                  | 0.49     | 0.05                | 0.48       |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB   | 19                  | 0.48     | 0.01                | 0.48       |
| (2,443)  | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 19                  | 0.46     | 0.11                | 0.5        |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23 | 19                  | 0.45     | 0.13                | 0.42       |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB  | 19                  | 0.44     | 0.13                | 0.48       |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB  | 19                  | 0.44     | 0.13                | 0.48       |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 19                  | 0.43     | 0.06                | 0.4        |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB   | 19                  | 0.41     | 0.11                | 0.43       |
| (1,333)  | 1:81:A:SER:HA  | 1:84:A:GLU:HB3  | 19                  | 0.39     | 0.07                | 0.41       |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA   | 19                  | 0.39     | 0.04                | 0.4        |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 19                  | 0.39     | 0.01                | 0.38       |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3  | 19                  | 0.38     | 0.11                | 0.39       |
| (1,970)  | 1:4:A:ILE:HB   | 1:6:A:HIS:HD2   | 19                  | 0.38     | 0.12                | 0.32       |
| (2,1099) | 1:120:A:PHE:H  | 1:32:A:ILE:CB   | 19                  | 0.37     | 0.09                | 0.35       |
| (2,241)  | 1:101:A:THR:CB | 1:100:A:SER:CB  | 19                  | 0.36     | 0.14                | 0.48       |
| (2,926)  | 1:101:A:THR:CB | 1:100:A:SER:CB  | 19                  | 0.36     | 0.14                | 0.48       |
| (1,173)  | 1:36:A:VAL:H   | 1:35:A:GLY:HA2  | 19                  | 0.32     | 0.06                | 0.35       |
| (1,359)  | 1:72:A:LEU:H   | 1:71:A:TYR:HB2  | 19                  | 0.29     | 0.06                | 0.28       |
| (2,645)  | 1:68:A:TYR:H   | 1:69:A:PHE:CB   | 19                  | 0.29     | 0.04                | 0.29       |
| (1,605)  | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 19                  | 0.23     | 0.03                | 0.23       |
| (1,1041) | 1:57:A:ASP:HA  | 1:58:A:GLY:H    | 19                  | 0.23     | 0.04                | 0.21       |
| (1,1210) | 1:43:A:GLY:H   | 1:92:A:VAL:HB   | 19                  | 0.2      | 0.03                | 0.2        |
| (1,702)  | 1:58:A:GLY:H   | 1:57:A:ASP:HB3  | 19                  | 0.17     | 0.03                | 0.19       |
| (2,177)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 19                  | 0.17     | 0.01                | 0.17       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,584)  | 1:108:A:ARG:CB  | 1:9:A:TRP:CB    | 18                  | 2.63     | 1.31                | 3.24       |
| (1,62)   | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 18                  | 2.11     | 0.39                | 2.18       |
| (2,956)  | 1:9:A:TRP:CB    | 1:107:A:SER:CB  | 18                  | 1.96     | 1.18                | 1.96       |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG   | 18                  | 1.51     | 0.57                | 1.82       |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 18                  | 1.5      | 0.75                | 1.46       |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 18                  | 1.4      | 0.27                | 1.43       |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 18                  | 1.03     | 0.32                | 1.06       |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 18                  | 0.92     | 0.75                | 0.84       |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 18                  | 0.9      | 0.13                | 0.88       |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 18                  | 0.83     | 0.26                | 0.76       |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 18                  | 0.83     | 0.18                | 0.9        |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB   | 18                  | 0.79     | 0.36                | 0.92       |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 18                  | 0.77     | 0.06                | 0.79       |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 18                  | 0.62     | 0.23                | 0.63       |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB   | 18                  | 0.54     | 0.3                 | 0.48       |
| (2,788)  | 1:92:A:VAL:H    | 1:90:A:PHE:CB   | 18                  | 0.53     | 0.1                 | 0.56       |
| (2,775)  | 1:28:A:GLN:H    | 1:25:A:SER:CB   | 18                  | 0.47     | 0.07                | 0.48       |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2  | 18                  | 0.45     | 0.08                | 0.43       |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 18                  | 0.44     | 0.26                | 0.34       |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 18                  | 0.38     | 0.11                | 0.4        |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 18                  | 0.38     | 0.11                | 0.4        |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2 | 18                  | 0.36     | 0.1                 | 0.39       |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 18                  | 0.31     | 0.03                | 0.3        |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 18                  | 0.31     | 0.03                | 0.3        |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 18                  | 0.3      | 0.11                | 0.27       |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 18                  | 0.2      | 0.05                | 0.2        |
| (1,93)   | 1:4:A:ILE:HB    | 1:5:A:PRO:HD3   | 18                  | 0.17     | 0.04                | 0.15       |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 17                  | 1.7      | 0.65                | 1.91       |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 17                  | 1.0      | 0.09                | 1.02       |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 17                  | 0.93     | 0.32                | 0.94       |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 17                  | 0.71     | 0.15                | 0.74       |
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 17                  | 0.69     | 0.33                | 0.67       |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 17                  | 0.65     | 0.28                | 0.57       |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 17                  | 0.59     | 0.24                | 0.59       |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 17                  | 0.41     | 0.23                | 0.3        |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 17                  | 0.23     | 0.05                | 0.22       |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 17                  | 0.17     | 0.07                | 0.16       |
| (1,509)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 17                  | 0.15     | 0.04                | 0.13       |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 17                  | 0.15     | 0.04                | 0.13       |
| (1,626)  | 1:89:A:VAL:HG13 | 1:86:A:LEU:HD21 | 17                  | 0.12     | 0.02                | 0.11       |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 16                  | 1.86     | 0.65                | 2.0        |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 16                  | 1.04     | 0.19                | 1.12       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1269) | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3  | 16                  | 0.88     | 0.22                | 0.9        |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2   | 16                  | 0.65     | 0.34                | 0.59       |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 16                  | 0.45     | 0.09                | 0.44       |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 16                  | 0.4      | 0.04                | 0.4        |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2   | 16                  | 0.36     | 0.19                | 0.32       |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3    | 16                  | 0.29     | 0.04                | 0.28       |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB    | 16                  | 0.28     | 0.1                 | 0.29       |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB    | 16                  | 0.26     | 0.09                | 0.26       |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB    | 16                  | 0.26     | 0.09                | 0.26       |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3   | 16                  | 0.21     | 0.05                | 0.2        |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 16                  | 0.2      | 0.08                | 0.21       |
| (1,924)  | 1:71:A:TYR:HD2  | 1:105:A:VAL:HG23 | 16                  | 0.18     | 0.1                 | 0.13       |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21  | 15                  | 1.37     | 0.23                | 1.46       |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB    | 15                  | 0.74     | 0.51                | 0.59       |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB    | 15                  | 0.74     | 0.51                | 0.59       |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB    | 15                  | 0.6      | 0.18                | 0.66       |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB    | 15                  | 0.59     | 0.27                | 0.52       |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB    | 15                  | 0.55     | 0.3                 | 0.7        |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2   | 15                  | 0.51     | 0.32                | 0.42       |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA    | 15                  | 0.35     | 0.12                | 0.32       |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 15                  | 0.35     | 0.19                | 0.31       |
| (1,78)   | 1:82:A:TYR:HB2  | 1:83:A:GLY:HA2   | 15                  | 0.34     | 0.07                | 0.36       |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 15                  | 0.25     | 0.06                | 0.27       |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 15                  | 0.25     | 0.06                | 0.27       |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23  | 15                  | 0.24     | 0.12                | 0.22       |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 15                  | 0.2      | 0.08                | 0.19       |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 15                  | 0.2      | 0.08                | 0.19       |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB    | 15                  | 0.19     | 0.05                | 0.2        |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1    | 14                  | 1.06     | 0.48                | 1.27       |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2   | 14                  | 1.0      | 0.57                | 0.85       |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2  | 14                  | 0.83     | 0.02                | 0.83       |
| (1,377)  | 1:11:A:SER:H    | 1:10:A:PHE:HB2   | 14                  | 0.52     | 0.11                | 0.51       |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB   | 14                  | 0.38     | 0.12                | 0.38       |
| (1,288)  | 1:16:A:PHE:HA   | 1:64:A:LEU:HD23  | 14                  | 0.31     | 0.21                | 0.29       |
| (2,718)  | 1:42:A:LYS:H    | 1:40:A:GLU:CB    | 14                  | 0.29     | 0.09                | 0.3        |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2  | 14                  | 0.25     | 0.04                | 0.23       |
| (1,888)  | 1:20:A:ARG:HD2  | 1:128:A:GLN:HG3  | 13                  | 1.62     | 1.06                | 1.11       |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3   | 13                  | 1.09     | 0.41                | 1.22       |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3   | 13                  | 1.06     | 0.34                | 1.23       |
| (2,188)  | 1:125:A:ILE:CB  | 1:23:A:LYS:CB    | 13                  | 0.77     | 0.32                | 0.82       |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB   | 13                  | 0.69     | 0.18                | 0.75       |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2  | 13                  | 0.68     | 0.24                | 0.69       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1216) | 1:100:A:SER:H    | 1:42:A:LYS:HE3   | 13                  | 0.63     | 0.08                | 0.64       |
| (1,1273) | 1:129:A:GLY:HA3  | 1:20:A:ARG:HG2   | 13                  | 0.37     | 0.18                | 0.34       |
| (1,33)   | 1:16:A:PHE:H     | 1:17:A:GLN:HB2   | 13                  | 0.28     | 0.07                | 0.28       |
| (1,343)  | 1:97:A:ALA:H     | 1:39:A:SER:HA    | 13                  | 0.26     | 0.09                | 0.27       |
| (2,945)  | 1:22:A:PHE:CA    | 1:127:A:PRO:CB   | 13                  | 0.22     | 0.08                | 0.23       |
| (2,74)   | 1:13:A:ILE:CA    | 1:133:A:GLU:H    | 13                  | 0.2      | 0.08                | 0.18       |
| (1,385)  | 1:118:A:THR:H    | 1:117:A:PRO:HB2  | 13                  | 0.18     | 0.06                | 0.17       |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 13                  | 0.17     | 0.12                | 0.13       |
| (2,920)  | 1:9:A:TRP:CB     | 1:108:A:ARG:CB   | 12                  | 1.31     | 0.34                | 1.22       |
| (2,1065) | 1:9:A:TRP:CB     | 1:108:A:ARG:CB   | 12                  | 1.31     | 0.34                | 1.22       |
| (2,1139) | 1:9:A:TRP:CB     | 1:108:A:ARG:CB   | 12                  | 1.31     | 0.34                | 1.22       |
| (1,1103) | 1:55:A:THR:H     | 1:54:A:LYS:HD3   | 12                  | 0.4      | 0.13                | 0.38       |
| (2,425)  | 1:132:A:VAL:H    | 1:126:A:LEU:CB   | 12                  | 0.34     | 0.12                | 0.34       |
| (2,1201) | 1:52:A:SER:CB    | 1:62:A:GLN:CB    | 12                  | 0.34     | 0.17                | 0.34       |
| (2,1200) | 1:130:A:TYR:CB   | 1:126:A:LEU:CB   | 12                  | 0.31     | 0.07                | 0.32       |
| (1,47)   | 1:25:A:SER:HA    | 1:28:A:GLN:HB3   | 12                  | 0.19     | 0.13                | 0.16       |
| (2,33)   | 1:104:A:ASP:H    | 1:105:A:VAL:CB   | 12                  | 0.17     | 0.05                | 0.17       |
| (1,1038) | 1:60:A:GLN:HB3   | 1:54:A:LYS:HE2   | 11                  | 0.87     | 0.24                | 0.94       |
| (1,1038) | 1:60:A:GLN:HB3   | 1:54:A:LYS:HE3   | 11                  | 0.87     | 0.24                | 0.94       |
| (1,86)   | 1:101:A:THR:HB   | 1:100:A:SER:HB3  | 11                  | 0.84     | 0.05                | 0.83       |
| (1,1121) | 1:130:A:TYR:H    | 1:127:A:PRO:HG3  | 11                  | 0.59     | 0.05                | 0.59       |
| (1,599)  | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD22  | 11                  | 0.5      | 0.42                | 0.28       |
| (1,1128) | 1:73:A:GLY:HA3   | 1:102:A:PRO:HG2  | 11                  | 0.34     | 0.22                | 0.28       |
| (2,369)  | 1:96:A:GLN:CB    | 1:38:A:PRO:CB    | 11                  | 0.28     | 0.15                | 0.3        |
| (1,771)  | 1:83:A:GLY:H     | 1:84:A:GLU:HB3   | 11                  | 0.28     | 0.12                | 0.21       |
| (2,440)  | 1:91:A:TRP:H     | 1:89:A:VAL:CB    | 11                  | 0.27     | 0.08                | 0.29       |
| (2,982)  | 1:124:A:THR:H    | 1:125:A:ILE:CB   | 11                  | 0.18     | 0.03                | 0.19       |
| (1,680)  | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 11                  | 0.17     | 0.1                 | 0.12       |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3   | 10                  | 0.43     | 0.22                | 0.35       |
| (1,384)  | 1:31:A:PRO:HB3   | 1:10:A:PHE:HE1   | 10                  | 0.27     | 0.12                | 0.26       |
| (1,384)  | 1:31:A:PRO:HB3   | 1:10:A:PHE:HE2   | 10                  | 0.27     | 0.12                | 0.26       |
| (1,284)  | 1:108:A:ARG:H    | 1:107:A:SER:H    | 10                  | 0.21     | 0.07                | 0.2        |
| (2,261)  | 1:108:A:ARG:H    | 1:107:A:SER:H    | 10                  | 0.21     | 0.07                | 0.2        |
| (2,885)  | 1:32:A:ILE:CB    | 1:120:A:PHE:CB   | 10                  | 0.17     | 0.07                | 0.15       |
| (2,79)   | 1:101:A:THR:CB   | 1:100:A:SER:CB   | 10                  | 0.16     | 0.01                | 0.16       |
| (2,657)  | 1:72:A:LEU:H     | 1:42:A:LYS:CB    | 10                  | 0.15     | 0.04                | 0.15       |
| (1,27)   | 1:60:A:GLN:HB3   | 1:54:A:LYS:HD2   | 9                   | 1.31     | 0.6                 | 1.63       |
| (1,29)   | 1:126:A:LEU:HA   | 1:125:A:ILE:HG12 | 9                   | 0.67     | 0.08                | 0.66       |
| (2,537)  | 1:124:A:THR:H    | 1:28:A:GLN:CB    | 9                   | 0.66     | 0.37                | 0.76       |
| (2,130)  | 1:120:A:PHE:CB   | 1:30:A:VAL:CA    | 9                   | 0.52     | 0.28                | 0.65       |
| (2,444)  | 1:104:A:ASP:CB   | 1:36:A:VAL:CB    | 9                   | 0.39     | 0.28                | 0.28       |
| (1,1016) | 1:126:A:LEU:H    | 1:125:A:ILE:HG12 | 9                   | 0.34     | 0.03                | 0.34       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (2,571)  | 1:89:A:VAL:CB    | 1:45:A:TRP:CB   | 9                   | 0.28     | 0.15                | 0.21       |
| (1,324)  | 1:73:A:GLY:H     | 1:74:A:THR:HB   | 9                   | 0.25     | 0.07                | 0.25       |
| (1,1211) | 1:43:A:GLY:H     | 1:72:A:LEU:HB3  | 9                   | 0.23     | 0.1                 | 0.19       |
| (1,221)  | 1:111:A:THR:H    | 1:110:A:PRO:HG3 | 9                   | 0.19     | 0.08                | 0.17       |
| (1,745)  | 1:91:A:TRP:H     | 1:90:A:PHE:HB3  | 9                   | 0.17     | 0.08                | 0.16       |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 8                   | 0.99     | 0.13                | 1.01       |
| (1,720)  | 1:70:A:TYR:H     | 1:31:A:PRO:HG2  | 8                   | 0.48     | 0.22                | 0.38       |
| (2,564)  | 1:127:A:PRO:CB   | 1:23:A:LYS:CB   | 8                   | 0.43     | 0.23                | 0.34       |
| (2,68)   | 1:86:A:LEU:H     | 1:45:A:TRP:CB   | 8                   | 0.35     | 0.19                | 0.29       |
| (1,1241) | 1:130:A:TYR:H    | 1:127:A:PRO:HB3 | 8                   | 0.33     | 0.11                | 0.33       |
| (1,1272) | 1:129:A:GLY:HA3  | 1:17:A:GLN:HB2  | 8                   | 0.31     | 0.21                | 0.24       |
| (2,749)  | 1:118:A:THR:CB   | 1:132:A:VAL:CB  | 8                   | 0.26     | 0.1                 | 0.22       |
| (2,865)  | 1:66:A:ARG:CB    | 1:68:A:TYR:CB   | 8                   | 0.24     | 0.13                | 0.19       |
| (2,887)  | 1:66:A:ARG:CB    | 1:68:A:TYR:CB   | 8                   | 0.24     | 0.13                | 0.19       |
| (2,685)  | 1:103:A:SER:H    | 1:105:A:VAL:CB  | 8                   | 0.22     | 0.1                 | 0.18       |
| (1,402)  | 1:32:A:ILE:HD12  | 1:121:A:PRO:HG2 | 8                   | 0.19     | 0.06                | 0.16       |
| (1,402)  | 1:32:A:ILE:HD11  | 1:121:A:PRO:HG2 | 8                   | 0.19     | 0.06                | 0.16       |
| (1,402)  | 1:32:A:ILE:HD13  | 1:121:A:PRO:HG2 | 8                   | 0.19     | 0.06                | 0.16       |
| (1,351)  | 1:130:A:TYR:H    | 1:129:A:GLY:HA2 | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1159) | 1:127:A:PRO:HA   | 1:128:A:GLN:HG3 | 8                   | 0.11     | 0.01                | 0.11       |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 7                   | 0.88     | 0.05                | 0.88       |
| (2,81)   | 1:9:A:TRP:CB     | 1:71:A:TYR:CB   | 7                   | 0.81     | 0.97                | 0.34       |
| (2,156)  | 1:4:A:ILE:CB     | 1:6:A:HIS:CB    | 7                   | 0.44     | 0.27                | 0.4        |
| (1,104)  | 1:108:A:ARG:H    | 1:106:A:SER:HA  | 7                   | 0.41     | 0.21                | 0.35       |
| (2,853)  | 1:6:A:HIS:CB     | 1:4:A:ILE:CB    | 7                   | 0.4      | 0.27                | 0.36       |
| (1,414)  | 1:65:A:PRO:HB3   | 1:67:A:TRP:HE1  | 7                   | 0.38     | 0.35                | 0.26       |
| (2,263)  | 1:16:A:PHE:CA    | 1:64:A:LEU:CB   | 7                   | 0.37     | 0.25                | 0.34       |
| (1,955)  | 1:13:A:ILE:HA    | 1:66:A:ARG:HG2  | 7                   | 0.35     | 0.2                 | 0.3        |
| (2,1126) | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 7                   | 0.28     | 0.13                | 0.25       |
| (2,697)  | 1:119:A:ARG:H    | 1:31:A:PRO:CB   | 7                   | 0.25     | 0.11                | 0.21       |
| (1,83)   | 1:46:A:TYR:HD1   | 1:76:A:PRO:HD3  | 7                   | 0.25     | 0.17                | 0.18       |
| (1,83)   | 1:46:A:TYR:HD2   | 1:76:A:PRO:HD3  | 7                   | 0.25     | 0.17                | 0.18       |
| (1,768)  | 1:119:A:ARG:H    | 1:31:A:PRO:HB3  | 7                   | 0.21     | 0.09                | 0.15       |
| (2,1112) | 1:121:A:PRO:CA   | 1:32:A:ILE:CB   | 7                   | 0.17     | 0.04                | 0.17       |
| (1,653)  | 1:16:A:PHE:H     | 1:64:A:LEU:HD21 | 7                   | 0.14     | 0.03                | 0.14       |
| (1,1228) | 1:103:A:SER:H    | 1:72:A:LEU:H    | 7                   | 0.12     | 0.01                | 0.13       |
| (2,1091) | 1:103:A:SER:H    | 1:72:A:LEU:H    | 7                   | 0.12     | 0.01                | 0.13       |
| (1,315)  | 1:74:A:THR:H     | 1:73:A:GLY:HA2  | 7                   | 0.12     | 0.02                | 0.12       |
| (2,1018) | 1:50:A:ARG:CB    | 1:66:A:ARG:CB   | 6                   | 1.04     | 0.45                | 1.11       |
| (1,363)  | 1:66:A:ARG:H     | 1:48:A:HIS:HB3  | 6                   | 0.62     | 0.17                | 0.56       |
| (1,941)  | 1:115:A:ALA:HA   | 1:114:A:GLU:HG2 | 6                   | 0.53     | 0.04                | 0.52       |
| (2,338)  | 1:66:A:ARG:H     | 1:48:A:HIS:CB   | 6                   | 0.4      | 0.14                | 0.4        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,281)  | 1:109:A:ASP:H   | 1:108:A:ARG:HB3 | 6                   | 0.38     | 0.15                | 0.34       |
| (2,705)  | 1:125:A:ILE:H   | 1:25:A:SER:CB   | 6                   | 0.29     | 0.17                | 0.28       |
| (2,654)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 6                   | 0.27     | 0.09                | 0.24       |
| (2,23)   | 1:115:A:ALA:H   | 1:114:A:GLU:CB  | 6                   | 0.24     | 0.05                | 0.24       |
| (2,560)  | 1:84:A:GLU:H    | 1:91:A:TRP:CB   | 6                   | 0.24     | 0.13                | 0.2        |
| (1,595)  | 1:115:A:ALA:HA  | 1:114:A:GLU:HB2 | 6                   | 0.22     | 0.06                | 0.22       |
| (2,987)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 6                   | 0.19     | 0.08                | 0.18       |
| (1,302)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:H    | 6                   | 0.18     | 0.06                | 0.18       |
| (1,81)   | 1:13:A:ILE:HA   | 1:133:A:GLU:H   | 6                   | 0.17     | 0.11                | 0.12       |
| (2,986)  | 1:102:A:PRO:CB  | 1:72:A:LEU:CB   | 6                   | 0.17     | 0.02                | 0.16       |
| (1,125)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG23  | 6                   | 0.14     | 0.02                | 0.14       |
| (2,538)  | 1:13:A:ILE:H    | 1:69:A:PHE:CB   | 6                   | 0.14     | 0.05                | 0.12       |
| (2,699)  | 1:111:A:THR:CB  | 1:110:A:PRO:CB  | 6                   | 0.14     | 0.03                | 0.14       |
| (1,1156) | 1:63:A:LEU:HA   | 1:62:A:GLN:HB2  | 6                   | 0.14     | 0.02                | 0.14       |
| (1,123)  | 1:22:A:PHE:H    | 1:21:A:ASP:HA   | 6                   | 0.13     | 0.02                | 0.14       |
| (1,854)  | 1:25:A:SER:H    | 1:29:A:GLY:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (2,777)  | 1:25:A:SER:H    | 1:29:A:GLY:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (2,237)  | 1:24:A:PHE:H    | 1:90:A:PHE:CB   | 5                   | 0.9      | 0.37                | 0.83       |
| (1,537)  | 1:54:A:LYS:HB2  | 1:60:A:GLN:HB3  | 5                   | 0.87     | 0.87                | 0.21       |
| (2,778)  | 1:29:A:GLY:H    | 1:120:A:PHE:CB  | 5                   | 0.71     | 0.72                | 0.37       |
| (1,785)  | 1:113:A:GLN:HG2 | 1:110:A:PRO:HB2 | 5                   | 0.7      | 0.38                | 0.71       |
| (2,164)  | 1:69:A:PHE:CB   | 1:10:A:PHE:CB   | 5                   | 0.5      | 0.25                | 0.52       |
| (1,39)   | 1:32:A:ILE:HG12 | 1:121:A:PRO:HG2 | 5                   | 0.5      | 0.05                | 0.51       |
| (1,533)  | 1:10:A:PHE:HB3  | 1:11:A:SER:HA   | 5                   | 0.36     | 0.04                | 0.35       |
| (2,404)  | 1:71:A:TYR:H    | 1:74:A:THR:CB   | 5                   | 0.34     | 0.15                | 0.29       |
| (2,128)  | 1:28:A:GLN:CA   | 1:120:A:PHE:CB  | 5                   | 0.33     | 0.28                | 0.26       |
| (2,1066) | 1:108:A:ARG:CA  | 1:9:A:TRP:CB    | 5                   | 0.3      | 0.12                | 0.27       |
| (1,201)  | 1:138:A:SER:H   | 1:137:A:ARG:HB2 | 5                   | 0.27     | 0.06                | 0.24       |
| (1,110)  | 1:32:A:ILE:HG23 | 1:121:A:PRO:HG2 | 5                   | 0.27     | 0.07                | 0.3        |
| (1,95)   | 1:34:A:PHE:HD2  | 1:71:A:TYR:HE1  | 5                   | 0.25     | 0.15                | 0.18       |
| (1,950)  | 1:8:A:SER:HB2   | 1:7:A:TYR:HA    | 5                   | 0.25     | 0.12                | 0.18       |
| (2,362)  | 1:104:A:ASP:H   | 1:40:A:GLU:CB   | 5                   | 0.2      | 0.08                | 0.15       |
| (1,109)  | 1:32:A:ILE:HG22 | 1:121:A:PRO:HG2 | 5                   | 0.19     | 0.04                | 0.2        |
| (1,109)  | 1:32:A:ILE:HG21 | 1:121:A:PRO:HG2 | 5                   | 0.19     | 0.04                | 0.2        |
| (1,138)  | 1:138:A:SER:H   | 1:137:A:ARG:HA  | 5                   | 0.18     | 0.05                | 0.19       |
| (1,712)  | 1:68:A:TYR:H    | 1:48:A:HIS:H    | 5                   | 0.18     | 0.09                | 0.14       |
| (2,643)  | 1:68:A:TYR:H    | 1:48:A:HIS:H    | 5                   | 0.18     | 0.09                | 0.14       |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD1 | 5                   | 0.17     | 0.04                | 0.18       |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD2 | 5                   | 0.17     | 0.04                | 0.18       |
| (1,491)  | 1:43:A:GLY:H    | 1:92:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (2,451)  | 1:43:A:GLY:H    | 1:92:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (2,152)  | 1:7:A:TYR:CB    | 1:110:A:PRO:CB  | 4                   | 0.77     | 0.32                | 0.86       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,944)  | 1:70:A:TYR:HB2   | 1:76:A:PRO:HD3   | 4                   | 0.64     | 0.2                 | 0.64       |
| (1,1140) | 1:50:A:ARG:HB3   | 1:66:A:ARG:HD2   | 4                   | 0.46     | 0.15                | 0.48       |
| (1,1140) | 1:50:A:ARG:HB2   | 1:66:A:ARG:HD2   | 4                   | 0.46     | 0.15                | 0.48       |
| (1,1199) | 1:9:A:TRP:HE1    | 1:108:A:ARG:HD3  | 4                   | 0.42     | 0.34                | 0.3        |
| (2,868)  | 1:4:A:ILE:CB     | 1:6:A:HIS:CB     | 4                   | 0.4      | 0.16                | 0.44       |
| (2,856)  | 1:6:A:HIS:CB     | 1:4:A:ILE:CB     | 4                   | 0.4      | 0.15                | 0.44       |
| (1,631)  | 1:89:A:VAL:HG23  | 1:86:A:LEU:HB3   | 4                   | 0.33     | 0.11                | 0.36       |
| (1,1011) | 1:42:A:LYS:HG2   | 1:72:A:LEU:HG    | 4                   | 0.22     | 0.07                | 0.18       |
| (1,874)  | 1:126:A:LEU:HB2  | 1:127:A:PRO:HD3  | 4                   | 0.19     | 0.06                | 0.2        |
| (2,1077) | 1:43:A:GLY:H     | 1:72:A:LEU:CB    | 4                   | 0.18     | 0.03                | 0.18       |
| (1,1252) | 1:121:A:PRO:HA   | 1:32:A:ILE:HG12  | 4                   | 0.17     | 0.03                | 0.16       |
| (1,6)    | 1:44:A:TYR:H     | 1:91:A:TRP:HZ3   | 4                   | 0.17     | 0.09                | 0.12       |
| (1,1120) | 1:130:A:TYR:H    | 1:13:A:ILE:HG23  | 4                   | 0.16     | 0.05                | 0.16       |
| (1,873)  | 1:78:A:ALA:H     | 1:76:A:PRO:HD3   | 4                   | 0.16     | 0.06                | 0.12       |
| (2,30)   | 1:16:A:PHE:H     | 1:17:A:GLN:CB    | 4                   | 0.14     | 0.02                | 0.14       |
| (1,927)  | 1:71:A:TYR:HE2   | 1:105:A:VAL:HG23 | 4                   | 0.14     | 0.03                | 0.13       |
| (1,1227) | 1:105:A:VAL:HA   | 1:103:A:SER:HB2  | 3                   | 1.04     | 0.07                | 1.08       |
| (1,736)  | 1:113:A:GLN:HA   | 1:108:A:ARG:HD2  | 3                   | 0.72     | 0.37                | 0.96       |
| (2,1148) | 1:64:A:LEU:CB    | 1:18:A:LYS:CB    | 3                   | 0.57     | 0.5                 | 0.25       |
| (2,1149) | 1:18:A:LYS:CB    | 1:64:A:LEU:CB    | 3                   | 0.57     | 0.5                 | 0.25       |
| (2,240)  | 1:20:A:ARG:H     | 1:17:A:GLN:CB    | 3                   | 0.53     | 0.17                | 0.55       |
| (1,456)  | 1:132:A:VAL:H    | 1:126:A:LEU:HD22 | 3                   | 0.48     | 0.08                | 0.43       |
| (1,469)  | 1:84:A:GLU:H     | 1:86:A:LEU:HD22  | 3                   | 0.46     | 0.02                | 0.47       |
| (1,654)  | 1:16:A:PHE:H     | 1:64:A:LEU:HD23  | 3                   | 0.43     | 0.22                | 0.47       |
| (1,477)  | 1:37:A:PRO:HD3   | 1:36:A:VAL:HG22  | 3                   | 0.4      | 0.01                | 0.4        |
| (1,477)  | 1:37:A:PRO:HD3   | 1:36:A:VAL:HG21  | 3                   | 0.4      | 0.01                | 0.4        |
| (1,263)  | 1:82:A:TYR:HA    | 1:83:A:GLY:H     | 3                   | 0.33     | 0.0                 | 0.33       |
| (1,805)  | 1:117:A:PRO:HA   | 1:11:A:SER:HA    | 3                   | 0.31     | 0.13                | 0.37       |
| (2,1087) | 1:137:A:ARG:H    | 1:11:A:SER:CB    | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,1277) | 1:15:A:GLN:HA    | 1:64:A:LEU:HB3   | 3                   | 0.28     | 0.1                 | 0.23       |
| (1,887)  | 1:129:A:GLY:HA3  | 1:128:A:GLN:HG3  | 3                   | 0.21     | 0.06                | 0.24       |
| (2,606)  | 1:32:A:ILE:CB    | 1:34:A:PHE:H     | 3                   | 0.21     | 0.1                 | 0.19       |
| (1,705)  | 1:73:A:GLY:HA3   | 1:102:A:PRO:HB2  | 3                   | 0.21     | 0.14                | 0.11       |
| (1,485)  | 1:40:A:GLU:HB3   | 1:36:A:VAL:HG23  | 3                   | 0.17     | 0.04                | 0.19       |
| (2,1116) | 1:82:A:TYR:CA    | 1:72:A:LEU:CB    | 3                   | 0.15     | 0.02                | 0.14       |
| (1,259)  | 1:10:A:PHE:HA    | 1:8:A:SER:HA     | 3                   | 0.15     | 0.04                | 0.12       |
| (1,508)  | 1:41:A:ALA:HA    | 1:71:A:TYR:HE2   | 3                   | 0.15     | 0.02                | 0.16       |
| (1,648)  | 1:15:A:GLN:H     | 1:13:A:ILE:HG23  | 3                   | 0.14     | 0.04                | 0.11       |
| (1,715)  | 1:105:A:VAL:HG12 | 1:103:A:SER:HB2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,715)  | 1:105:A:VAL:HG11 | 1:103:A:SER:HB2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,715)  | 1:105:A:VAL:HG13 | 1:103:A:SER:HB2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,257)  | 1:116:A:ILE:HG23 | 1:10:A:PHE:HA    | 3                   | 0.11     | 0.01                | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1013) | 1:64:A:LEU:H     | 1:63:A:LEU:HG    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,120)  | 1:24:A:PHE:HA    | 1:125:A:ILE:HG23 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,347)  | 1:89:A:VAL:H     | 1:88:A:GLY:HA3   | 3                   | 0.11     | 0.01                | 0.1        |
| (1,473)  | 1:86:A:LEU:H     | 1:89:A:VAL:HG12  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,473)  | 1:86:A:LEU:H     | 1:89:A:VAL:HG11  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,473)  | 1:86:A:LEU:H     | 1:89:A:VAL:HG13  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,652)  | 1:16:A:PHE:H     | 1:64:A:LEU:HD22  | 2                   | 1.19     | 0.05                | 1.19       |
| (1,482)  | 1:104:A:ASP:HB3  | 1:36:A:VAL:HG23  | 2                   | 0.88     | 0.01                | 0.88       |
| (1,788)  | 1:20:A:ARG:HB3   | 1:17:A:GLN:HE22  | 2                   | 0.67     | 0.4                 | 0.67       |
| (1,286)  | 1:16:A:PHE:HA    | 1:64:A:LEU:HD22  | 2                   | 0.66     | 0.03                | 0.66       |
| (2,627)  | 1:52:A:SER:H     | 1:63:A:LEU:CB    | 2                   | 0.58     | 0.02                | 0.58       |
| (2,1043) | 1:52:A:SER:H     | 1:63:A:LEU:CB    | 2                   | 0.58     | 0.02                | 0.58       |
| (1,1173) | 1:51:A:ARG:HB2   | 1:63:A:LEU:HD21  | 2                   | 0.34     | 0.16                | 0.34       |
| (1,1266) | 1:51:A:ARG:HB2   | 1:63:A:LEU:HD21  | 2                   | 0.34     | 0.16                | 0.34       |
| (1,1104) | 1:52:A:SER:HA    | 1:51:A:ARG:HG2   | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,1029) | 1:51:A:ARG:HA    | 1:63:A:LEU:HD21  | 2                   | 0.34     | 0.02                | 0.34       |
| (2,497)  | 1:54:A:LYS:CB    | 1:60:A:GLN:CB    | 2                   | 0.3      | 0.08                | 0.3        |
| (1,155)  | 1:106:A:SER:H    | 1:105:A:VAL:HA   | 2                   | 0.3      | 0.01                | 0.3        |
| (1,794)  | 1:114:A:GLU:HG2  | 1:115:A:ALA:HB2  | 2                   | 0.27     | 0.01                | 0.27       |
| (1,794)  | 1:114:A:GLU:HG2  | 1:115:A:ALA:HB1  | 2                   | 0.27     | 0.01                | 0.27       |
| (1,794)  | 1:114:A:GLU:HG2  | 1:115:A:ALA:HB3  | 2                   | 0.27     | 0.01                | 0.27       |
| (1,1017) | 1:29:A:GLY:H     | 1:28:A:GLN:HB3   | 2                   | 0.26     | 0.04                | 0.26       |
| (2,217)  | 1:89:A:VAL:CB    | 1:45:A:TRP:CB    | 2                   | 0.26     | 0.1                 | 0.26       |
| (2,24)   | 1:60:A:GLN:CB    | 1:54:A:LYS:CB    | 2                   | 0.24     | 0.08                | 0.24       |
| (1,521)  | 1:118:A:THR:H    | 1:11:A:SER:H     | 2                   | 0.22     | 0.08                | 0.22       |
| (2,481)  | 1:118:A:THR:H    | 1:11:A:SER:H     | 2                   | 0.22     | 0.08                | 0.22       |
| (2,385)  | 1:16:A:PHE:H     | 1:64:A:LEU:CB    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,276)  | 1:112:A:THR:H    | 1:109:A:ASP:H    | 2                   | 0.21     | 0.1                 | 0.21       |
| (2,255)  | 1:112:A:THR:H    | 1:109:A:ASP:H    | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,114)  | 1:104:A:ASP:H    | 1:103:A:SER:HA   | 2                   | 0.2      | 0.06                | 0.2        |
| (1,621)  | 1:89:A:VAL:HG12  | 1:86:A:LEU:HD22  | 2                   | 0.19     | 0.07                | 0.19       |
| (1,1014) | 1:62:A:GLN:HA    | 1:52:A:SER:HA    | 2                   | 0.19     | 0.05                | 0.19       |
| (2,536)  | 1:79:A:ASN:CA    | 1:72:A:LEU:CB    | 2                   | 0.18     | 0.01                | 0.18       |
| (1,152)  | 1:114:A:GLU:HA   | 1:115:A:ALA:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1261) | 1:7:A:TYR:H      | 1:6:A:HIS:HB2    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,355)  | 1:82:A:TYR:H     | 1:81:A:SER:HB3   | 2                   | 0.16     | 0.02                | 0.16       |
| (2,635)  | 1:59:A:GLN:H     | 1:54:A:LYS:CB    | 2                   | 0.15     | 0.03                | 0.15       |
| (1,416)  | 1:97:A:ALA:H     | 1:96:A:GLN:HB3   | 2                   | 0.14     | 0.04                | 0.14       |
| (1,121)  | 1:68:A:TYR:HE1   | 1:66:A:ARG:HB2   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,121)  | 1:68:A:TYR:HE2   | 1:66:A:ARG:HB2   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1220) | 1:103:A:SER:HA   | 1:72:A:LEU:HD21  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,87)   | 1:113:A:GLN:HE21 | 1:9:A:TRP:HD1    | 2                   | 0.13     | 0.0                 | 0.13       |

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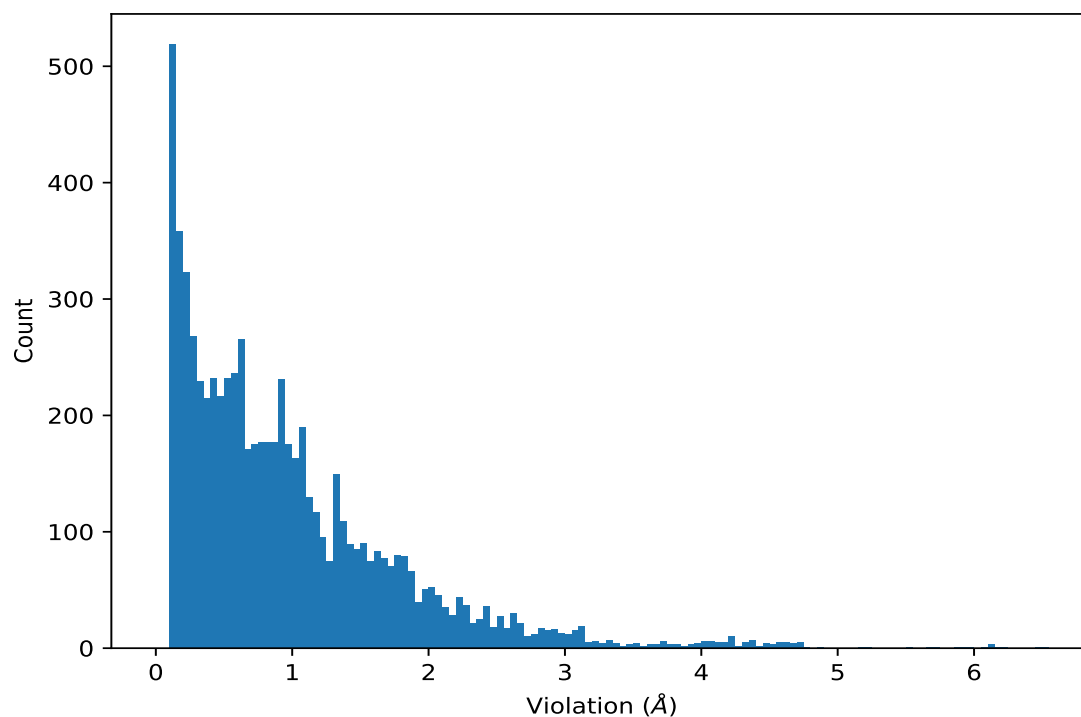
| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,833)  | 1:118:A:THR:H  | 1:117:A:PRO:HG2 | 2                   | 0.13     | 0.01                | 0.13       |
| (2,980)  | 1:124:A:THR:H  | 1:28:A:GLN:CB   | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1008) | 1:116:A:ILE:HA | 1:117:A:PRO:HD2 | 2                   | 0.12     | 0.02                | 0.12       |
| (2,361)  | 1:81:A:SER:H   | 1:84:A:GLU:CB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,19)   | 1:77:A:TYR:H   | 1:76:A:PRO:HG3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,829)  | 1:101:A:THR:H  | 1:98:A:ASP:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (2,754)  | 1:101:A:THR:H  | 1:98:A:ASP: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) |
|---------|----------------|----------------|----------|---------------|
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 14       | 6.55          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 5        | 6.48          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 13       | 6.21          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 2        | 6.17          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 9        | 6.13          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 3        | 6.12          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 6        | 6.11          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 10       | 6.08          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 7        | 5.96          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 17       | 5.93          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 15       | 5.88          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 19       | 5.7           |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 4        | 5.65          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 16       | 5.51          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 8        | 5.22          |
| (2,829) | 1:9:A:TRP:CB   | 1:105:A:VAL:CB | 17       | 5.18          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 4        | 4.87          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 15       | 4.78          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 1        | 4.74          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 12       | 4.73          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 15       | 4.73          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 1        | 4.72          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 11       | 4.71          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 14       | 4.68          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 19       | 4.68          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 10       | 4.66          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 17       | 4.65          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 16       | 4.62          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 3        | 4.61          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 18       | 4.61          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 12       | 4.61          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 6        | 4.6           |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 13       | 4.59          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 18       | 4.59          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 4        | 4.58          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 7        | 4.57          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 6        | 4.56          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 2        | 4.53          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 8        | 4.51          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 7        | 4.5           |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 5        | 4.48          |
| (2,286) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 9        | 4.46          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 1        | 4.45          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 12       | 4.45          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 15       | 4.44          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 11       | 4.42          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 14       | 4.39          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 19       | 4.39          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 10       | 4.38          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 17       | 4.37          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 4        | 4.36          |
| (2,88)  | 1:34:A:PHE:CB  | 1:71:A:TYR:CB  | 11       | 4.36          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 14       | 4.36          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 16       | 4.33          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 3        | 4.32          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 6        | 4.32          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 18       | 4.32          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 13       | 4.31          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 8        | 4.29          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 8        | 4.29          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 2        | 4.24          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 1        | 4.23          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 7        | 4.22          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 8        | 4.22          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 12       | 4.22          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 15       | 4.22          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 4        | 4.22          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 9        | 4.21          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 5        | 4.2           |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 11       | 4.2           |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 5        | 4.19          |
| (2,937) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 9        | 4.18          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 14       | 4.17          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 19       | 4.17          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 10       | 4.16          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 17       | 4.14          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 16       | 4.11          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 3        | 4.1           |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 18       | 4.1           |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 3        | 4.1           |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 6        | 4.09          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 13       | 4.09          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 4        | 4.08          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 11       | 4.06          |
| (2,956) | 1:9:A:TRP:CB   | 1:107:A:SER:CB | 1        | 4.05          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 10       | 4.05          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 16       | 4.04          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 5        | 4.03          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 2        | 4.02          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 14       | 4.02          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 7        | 4.0           |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 8        | 4.0           |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 4        | 3.99          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 5        | 3.98          |
| (2,878) | 1:91:A:TRP:CB  | 1:72:A:LEU:CB  | 9        | 3.95          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 14       | 3.95          |
| (2,689) | 1:106:A:SER:H  | 1:9:A:TRP:CB   | 17       | 3.94          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 13       | 3.93          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 18       | 3.91          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 5        | 3.89          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 17       | 3.86          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 7        | 3.83          |
| (2,956) | 1:9:A:TRP:CB   | 1:107:A:SER:CB | 15       | 3.81          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 9        | 3.8           |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 6        | 3.79          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 11       | 3.75          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 13       | 3.75          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 2        | 3.74          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 10       | 3.72          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 19       | 3.71          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 14       | 3.7           |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 15       | 3.7           |
| (2,583) | 1:105:A:VAL:CB | 1:9:A:TRP:CB   | 17       | 3.7           |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 11       | 3.69          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 10       | 3.68          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB  | 8        | 3.66          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 1        | 3.64          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 12       | 3.62          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 9        | 3.62          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 2        | 3.58          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB  | 17       | 3.55          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 3        | 3.54          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 2        | 3.53          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 1        | 3.51          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 3        | 3.51          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 7        | 3.47          |
| (2,956) | 1:9:A:TRP:CB   | 1:107:A:SER:CB | 16       | 3.45          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 11       | 3.45          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 16       | 3.43          |
| (2,781) | 1:124:A:THR:CB | 1:127:A:PRO:CB | 8        | 3.42          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB  | 16       | 3.39          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 17       | 3.37          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 19       | 3.37          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 10       | 3.36          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 8        | 3.34          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 11       | 3.34          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 6        | 3.33          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 10       | 3.33          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB  | 4        | 3.32          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 4        | 3.3           |
| (1,373) | 1:96:A:GLN:H   | 1:94:A:ASN:HB2 | 3        | 3.3           |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 16       | 3.29          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 18       | 3.28          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 13       | 3.27          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 9        | 3.26          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 5        | 3.24          |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 5        | 3.22          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 14       | 3.22          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 7        | 3.21          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 4        | 3.2           |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 4        | 3.2           |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 19       | 3.19          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 6        | 3.17          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB  | 2        | 3.17          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 8        | 3.17          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 15       | 3.17          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 17       | 3.14          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 19       | 3.14          |
| (2,514) | 1:108:A:ARG:H  | 1:9:A:TRP:CB   | 16       | 3.14          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 2        | 3.14          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 17       | 3.14          |
| (2,81)  | 1:9:A:TRP:CB   | 1:71:A:TYR:CB  | 17       | 3.14          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 2        | 3.13          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 15       | 3.13          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 8        | 3.12          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 11       | 3.12          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 16       | 3.12          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 11       | 3.12          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 10       | 3.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 18       | 3.11          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 3        | 3.11          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB   | 19       | 3.11          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 6        | 3.1           |
| (2,728) | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 1        | 3.1           |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 18       | 3.1           |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB  | 17       | 3.08          |
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB  | 17       | 3.08          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 12       | 3.08          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 16       | 3.07          |
| (2,514) | 1:108:A:ARG:H  | 1:9:A:TRP:CB   | 1        | 3.07          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 11       | 3.07          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 15       | 3.07          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 19       | 3.07          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 3        | 3.06          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 18       | 3.06          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 14       | 3.06          |
| (2,956) | 1:9:A:TRP:CB   | 1:107:A:SER:CB | 13       | 3.05          |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB  | 8        | 3.05          |
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB  | 8        | 3.05          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 2        | 3.05          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 9        | 3.04          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 13       | 3.04          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 7        | 3.04          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 12       | 3.04          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 7        | 3.04          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 9        | 3.04          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 1        | 3.03          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 5        | 3.02          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB | 3        | 3.02          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 6        | 3.02          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 16       | 3.01          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 14       | 3.0           |
| (2,514) | 1:108:A:ARG:H  | 1:9:A:TRP:CB   | 7        | 2.99          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB  | 19       | 2.99          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 5        | 2.99          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 7        | 2.98          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB  | 1        | 2.98          |
| (2,584) | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 12       | 2.97          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB  | 1        | 2.97          |
| (2,956) | 1:9:A:TRP:CB   | 1:107:A:SER:CB | 9        | 2.96          |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB  | 19       | 2.96          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 19       | 2.96          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 6        | 2.96          |
| (2,846) | 1:70:A:TYR:CB  | 1:76:A:PRO:CB   | 17       | 2.95          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB   | 12       | 2.95          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 13       | 2.94          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 10       | 2.94          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 12       | 2.94          |
| (2,829) | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 9        | 2.92          |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 10       | 2.92          |
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 10       | 2.92          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 13       | 2.92          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB   | 10       | 2.92          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 2        | 2.91          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 15       | 2.91          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 2        | 2.91          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 4        | 2.91          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 5        | 2.9           |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 9        | 2.9           |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 11       | 2.9           |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 15       | 2.9           |
| (2,956) | 1:9:A:TRP:CB   | 1:107:A:SER:CB  | 18       | 2.89          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 18       | 2.89          |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 11       | 2.89          |
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 11       | 2.89          |
| (1,888) | 1:20:A:ARG:HD2 | 1:128:A:GLN:HG3 | 8        | 2.89          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 10       | 2.88          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 14       | 2.88          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 15       | 2.88          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 5        | 2.88          |
| (2,582) | 1:107:A:SER:CA | 1:9:A:TRP:CB    | 1        | 2.87          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 17       | 2.87          |
| (2,879) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 12       | 2.86          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 9        | 2.86          |
| (2,468) | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 3        | 2.85          |
| (2,87)  | 1:46:A:TYR:CB  | 1:44:A:TYR:CB   | 13       | 2.85          |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 5        | 2.84          |
| (2,750) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 7        | 2.84          |
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 5        | 2.84          |
| (2,573) | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 7        | 2.84          |
| (2,548) | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 4        | 2.84          |
| (2,514) | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 6        | 2.84          |
| (2,243) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 14       | 2.84          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,243)  | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 16       | 2.84          |
| (2,879)  | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 3        | 2.83          |
| (2,378)  | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 6        | 2.83          |
| (2,243)  | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 18       | 2.83          |
| (2,243)  | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 6        | 2.82          |
| (2,171)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 19       | 2.82          |
| (2,750)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 14       | 2.81          |
| (2,573)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 14       | 2.81          |
| (2,514)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 18       | 2.81          |
| (2,846)  | 1:70:A:TYR:CB  | 1:76:A:PRO:CB   | 14       | 2.8           |
| (2,833)  | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 6        | 2.78          |
| (2,378)  | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 3        | 2.78          |
| (2,378)  | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 19       | 2.78          |
| (2,243)  | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 1        | 2.78          |
| (2,243)  | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 8        | 2.78          |
| (2,750)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 9        | 2.77          |
| (2,573)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 9        | 2.77          |
| (2,514)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 4        | 2.77          |
| (2,378)  | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 11       | 2.77          |
| (2,80)   | 1:113:A:GLN:CB | 1:9:A:TRP:CB    | 15       | 2.77          |
| (2,514)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 5        | 2.76          |
| (2,879)  | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 1        | 2.75          |
| (2,468)  | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 17       | 2.74          |
| (2,260)  | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 3        | 2.74          |
| (2,378)  | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 13       | 2.72          |
| (2,182)  | 1:18:A:LYS:CB  | 1:64:A:LEU:CB   | 10       | 2.72          |
| (1,888)  | 1:20:A:ARG:HD2 | 1:128:A:GLN:HG3 | 15       | 2.71          |
| (2,750)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 12       | 2.7           |
| (2,750)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 18       | 2.7           |
| (2,573)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 12       | 2.7           |
| (2,573)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 18       | 2.7           |
| (1,888)  | 1:20:A:ARG:HD2 | 1:128:A:GLN:HG3 | 14       | 2.7           |
| (2,468)  | 1:41:A:ALA:CA  | 1:71:A:TYR:CB   | 8        | 2.69          |
| (2,243)  | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 19       | 2.69          |
| (1,1363) | 1:52:A:SER:HB2 | 1:62:A:GLN:HG2  | 11       | 2.69          |
| (2,750)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 2        | 2.68          |
| (2,750)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 13       | 2.68          |
| (2,573)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 2        | 2.68          |
| (2,573)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 13       | 2.68          |
| (2,171)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 4        | 2.68          |
| (2,750)  | 1:80:A:ALA:H   | 1:91:A:TRP:CB   | 15       | 2.67          |
| (2,582)  | 1:107:A:SER:CA | 1:9:A:TRP:CB    | 15       | 2.67          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,573) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 15       | 2.67          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 10       | 2.67          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 17       | 2.67          |
| (1,888) | 1:20:A:ARG:HD2  | 1:128:A:GLN:HG3 | 13       | 2.67          |
| (2,514) | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 12       | 2.66          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 12       | 2.66          |
| (2,80)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CB    | 7        | 2.66          |
| (1,888) | 1:20:A:ARG:HD2  | 1:128:A:GLN:HG3 | 6        | 2.66          |
| (2,846) | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 9        | 2.65          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 1        | 2.65          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 1        | 2.65          |
| (2,750) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 1        | 2.64          |
| (2,750) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 3        | 2.64          |
| (2,573) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 1        | 2.64          |
| (2,573) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 3        | 2.64          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 2        | 2.64          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 4        | 2.64          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 13       | 2.64          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 17       | 2.64          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 19       | 2.64          |
| (2,750) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 6        | 2.63          |
| (2,573) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 6        | 2.63          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 15       | 2.63          |
| (2,243) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 7        | 2.63          |
| (2,846) | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 8        | 2.62          |
| (2,662) | 1:78:A:ALA:H    | 1:44:A:TYR:CB   | 19       | 2.62          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 11       | 2.62          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 16       | 2.62          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 8        | 2.62          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 11       | 2.62          |
| (1,888) | 1:20:A:ARG:HD2  | 1:128:A:GLN:HG3 | 16       | 2.62          |
| (1,607) | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 4        | 2.62          |
| (1,62)  | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 11       | 2.62          |
| (2,879) | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 4        | 2.61          |
| (2,662) | 1:78:A:ALA:H    | 1:44:A:TYR:CB   | 18       | 2.61          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 10       | 2.61          |
| (2,514) | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 2        | 2.6           |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 5        | 2.6           |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 17       | 2.6           |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 6        | 2.6           |
| (1,607) | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 16       | 2.6           |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 9        | 2.59          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,171) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 10       | 2.59          |
| (2,829) | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 2        | 2.58          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 7        | 2.58          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 10       | 2.58          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 1        | 2.58          |
| (2,171) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 5        | 2.58          |
| (2,80)  | 1:113:A:GLN:CB | 1:9:A:TRP:CB    | 16       | 2.58          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 11       | 2.57          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 9        | 2.56          |
| (2,260) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 14       | 2.56          |
| (2,260) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 16       | 2.56          |
| (2,260) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 18       | 2.56          |
| (2,42)  | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 16       | 2.56          |
| (2,829) | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 8        | 2.55          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 10       | 2.55          |
| (2,260) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 6        | 2.55          |
| (2,378) | 1:84:A:GLU:CB  | 1:45:A:TRP:CB   | 7        | 2.54          |
| (2,226) | 1:113:A:GLN:CB | 1:9:A:TRP:CA    | 14       | 2.54          |
| (2,42)  | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 9        | 2.54          |
| (2,42)  | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 13       | 2.54          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 3        | 2.53          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 4        | 2.53          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 15       | 2.53          |
| (1,62)  | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 2        | 2.53          |
| (2,935) | 1:42:A:LYS:CB  | 1:98:A:ASP:CB   | 12       | 2.52          |
| (2,829) | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 18       | 2.52          |
| (2,827) | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 9        | 2.52          |
| (2,827) | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 9        | 2.52          |
| (2,800) | 1:126:A:LEU:CB | 1:13:A:ILE:CB   | 3        | 2.52          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 14       | 2.52          |
| (2,437) | 1:84:A:GLU:H   | 1:86:A:LEU:CB   | 15       | 2.52          |
| (2,829) | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 12       | 2.51          |
| (2,689) | 1:106:A:SER:H  | 1:9:A:TRP:CB    | 9        | 2.51          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 6        | 2.51          |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 12       | 2.51          |
| (2,514) | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 15       | 2.51          |
| (2,171) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 1        | 2.51          |
| (2,42)  | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 5        | 2.51          |
| (2,818) | 1:132:A:VAL:CB | 1:118:A:THR:CB  | 10       | 2.5           |
| (2,662) | 1:78:A:ALA:H   | 1:44:A:TYR:CB   | 9        | 2.5           |
| (2,260) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 1        | 2.5           |
| (2,260) | 1:13:A:ILE:CB  | 1:126:A:LEU:CB  | 8        | 2.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 14       | 2.5           |
| (2,829) | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 10       | 2.49          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 12       | 2.49          |
| (2,662) | 1:78:A:ALA:H    | 1:44:A:TYR:CB   | 1        | 2.48          |
| (2,378) | 1:84:A:GLU:CB   | 1:45:A:TRP:CB   | 12       | 2.48          |
| (2,226) | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 8        | 2.48          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 7        | 2.48          |
| (2,662) | 1:78:A:ALA:H    | 1:44:A:TYR:CB   | 5        | 2.47          |
| (2,662) | 1:78:A:ALA:H    | 1:44:A:TYR:CB   | 13       | 2.47          |
| (2,388) | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 11       | 2.47          |
| (2,80)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CB    | 12       | 2.47          |
| (2,818) | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 12       | 2.46          |
| (2,750) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 16       | 2.46          |
| (2,573) | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 16       | 2.46          |
| (2,388) | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 10       | 2.46          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 15       | 2.46          |
| (2,514) | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 14       | 2.45          |
| (1,607) | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 17       | 2.45          |
| (1,62)  | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 8        | 2.45          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 10       | 2.44          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 3        | 2.44          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 4        | 2.44          |
| (2,35)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 19       | 2.44          |
| (1,62)  | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 13       | 2.44          |
| (2,829) | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 7        | 2.43          |
| (2,818) | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 4        | 2.43          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 12       | 2.43          |
| (1,62)  | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 12       | 2.43          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 14       | 2.42          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 14       | 2.42          |
| (2,437) | 1:84:A:GLU:H    | 1:86:A:LEU:CB   | 19       | 2.42          |
| (2,260) | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 19       | 2.42          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 2        | 2.42          |
| (2,833) | 1:13:A:ILE:CB   | 1:120:A:PHE:CB  | 8        | 2.41          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 2        | 2.41          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 4        | 2.41          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 13       | 2.41          |
| (2,582) | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 16       | 2.41          |
| (2,558) | 1:84:A:GLU:CB   | 1:86:A:LEU:CB   | 15       | 2.41          |
| (2,388) | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 15       | 2.41          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 14       | 2.41          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 8        | 2.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 15       | 2.41          |
| (2,42)   | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 2        | 2.41          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 10       | 2.41          |
| (2,800)  | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 11       | 2.4           |
| (2,800)  | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 15       | 2.4           |
| (2,750)  | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 4        | 2.4           |
| (2,573)  | 1:80:A:ALA:H    | 1:91:A:TRP:CB   | 4        | 2.4           |
| (2,378)  | 1:84:A:GLU:CB   | 1:45:A:TRP:CB   | 8        | 2.4           |
| (2,378)  | 1:84:A:GLU:CB   | 1:45:A:TRP:CB   | 14       | 2.4           |
| (2,378)  | 1:84:A:GLU:CB   | 1:45:A:TRP:CB   | 18       | 2.4           |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 4        | 2.4           |
| (2,42)   | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 15       | 2.4           |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 19       | 2.4           |
| (2,935)  | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 11       | 2.39          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 1        | 2.39          |
| (2,42)   | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 18       | 2.39          |
| (1,308)  | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 2        | 2.39          |
| (2,935)  | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 4        | 2.38          |
| (2,662)  | 1:78:A:ALA:H    | 1:44:A:TYR:CB   | 2        | 2.38          |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 2        | 2.38          |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 17       | 2.38          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 8        | 2.38          |
| (1,308)  | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 7        | 2.38          |
| (2,829)  | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 5        | 2.37          |
| (2,800)  | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 5        | 2.37          |
| (2,800)  | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 17       | 2.37          |
| (2,662)  | 1:78:A:ALA:H    | 1:44:A:TYR:CB   | 16       | 2.37          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 19       | 2.36          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 7        | 2.36          |
| (2,800)  | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 9        | 2.36          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 18       | 2.36          |
| (2,260)  | 1:13:A:ILE:CB   | 1:126:A:LEU:CB  | 7        | 2.36          |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 11       | 2.36          |
| (2,42)   | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 12       | 2.36          |
| (2,935)  | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 5        | 2.35          |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 3        | 2.35          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 5        | 2.35          |
| (1,62)   | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 14       | 2.35          |
| (2,866)  | 1:41:A:ALA:CB   | 1:71:A:TYR:CB   | 4        | 2.34          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 19       | 2.34          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 3        | 2.34          |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 18       | 2.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 14       | 2.33          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 16       | 2.33          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 18       | 2.33          |
| (2,388) | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 13       | 2.33          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 13       | 2.33          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 3        | 2.33          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 10       | 2.32          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 14       | 2.32          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 15       | 2.32          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 6        | 2.32          |
| (2,728) | 1:113:A:GLN:CB  | 1:116:A:ILE:CB  | 2        | 2.32          |
| (1,607) | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 6        | 2.32          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 19       | 2.31          |
| (1,308) | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 4        | 2.31          |
| (2,818) | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 17       | 2.3           |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 14       | 2.3           |
| (2,35)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 4        | 2.3           |
| (2,846) | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 11       | 2.29          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 8        | 2.29          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 8        | 2.29          |
| (2,818) | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 5        | 2.29          |
| (2,388) | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 7        | 2.29          |
| (2,358) | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 12       | 2.29          |
| (2,35)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 17       | 2.29          |
| (1,308) | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 14       | 2.29          |
| (1,62)  | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 9        | 2.29          |
| (2,818) | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 3        | 2.28          |
| (2,582) | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 18       | 2.28          |
| (2,376) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 19       | 2.28          |
| (2,347) | 1:96:A:GLN:H    | 1:94:A:ASN:CB   | 3        | 2.28          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 7        | 2.28          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 9        | 2.28          |
| (2,6)   | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 8        | 2.28          |
| (1,62)  | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 18       | 2.28          |
| (2,956) | 1:9:A:TRP:CB    | 1:107:A:SER:CB  | 3        | 2.27          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 7        | 2.27          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 18       | 2.27          |
| (2,833) | 1:13:A:ILE:CB   | 1:120:A:PHE:CB  | 17       | 2.27          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 1        | 2.27          |
| (2,800) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 8        | 2.27          |
| (2,226) | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 5        | 2.27          |
| (1,308) | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 11       | 2.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 13       | 2.26          |
| (2,829) | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 15       | 2.26          |
| (2,437) | 1:84:A:GLU:H    | 1:86:A:LEU:CB   | 12       | 2.26          |
| (2,378) | 1:84:A:GLU:CB   | 1:45:A:TRP:CB   | 17       | 2.26          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 6        | 2.26          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 1        | 2.25          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 11       | 2.25          |
| (2,827) | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 11       | 2.25          |
| (2,728) | 1:113:A:GLN:CB  | 1:116:A:ILE:CB  | 18       | 2.25          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 16       | 2.25          |
| (2,42)  | 1:80:A:ALA:CB   | 1:91:A:TRP:CB   | 1        | 2.25          |
| (1,607) | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 7        | 2.25          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 17       | 2.24          |
| (2,833) | 1:13:A:ILE:CB   | 1:120:A:PHE:CB  | 1        | 2.24          |
| (2,818) | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 9        | 2.24          |
| (2,818) | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 15       | 2.24          |
| (2,761) | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 16       | 2.24          |
| (2,437) | 1:84:A:GLU:H    | 1:86:A:LEU:CB   | 14       | 2.24          |
| (2,388) | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 17       | 2.24          |
| (2,35)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 16       | 2.24          |
| (1,308) | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 5        | 2.24          |
| (1,308) | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 9        | 2.24          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 2        | 2.23          |
| (2,866) | 1:41:A:ALA:CB   | 1:71:A:TYR:CB   | 16       | 2.23          |
| (2,846) | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 2        | 2.23          |
| (2,833) | 1:13:A:ILE:CB   | 1:120:A:PHE:CB  | 14       | 2.23          |
| (2,514) | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 10       | 2.23          |
| (2,226) | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 9        | 2.23          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 6        | 2.23          |
| (2,171) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 8        | 2.23          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 5        | 2.23          |
| (1,308) | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 3        | 2.23          |
| (1,62)  | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 3        | 2.23          |
| (2,989) | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 4        | 2.22          |
| (2,833) | 1:13:A:ILE:CB   | 1:120:A:PHE:CB  | 4        | 2.22          |
| (2,388) | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 6        | 2.22          |
| (2,83)  | 1:44:A:TYR:CB   | 1:46:A:TYR:CB   | 1        | 2.22          |
| (1,308) | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3  | 8        | 2.22          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 3        | 2.21          |
| (2,935) | 1:42:A:LYS:CB   | 1:98:A:ASP:CB   | 9        | 2.21          |
| (2,728) | 1:113:A:GLN:CB  | 1:116:A:ILE:CB  | 17       | 2.21          |
| (2,641) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 13       | 2.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,558)  | 1:84:A:GLU:CB   | 1:86:A:LEU:CB  | 4        | 2.21          |
| (2,80)   | 1:113:A:GLN:CB  | 1:9:A:TRP:CB   | 6        | 2.21          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 17       | 2.2           |
| (2,935)  | 1:42:A:LYS:CB   | 1:98:A:ASP:CB  | 6        | 2.2           |
| (2,866)  | 1:41:A:ALA:CB   | 1:71:A:TYR:CB  | 19       | 2.2           |
| (2,833)  | 1:13:A:ILE:CB   | 1:120:A:PHE:CB | 10       | 2.2           |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB | 5        | 2.2           |
| (2,514)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB   | 11       | 2.2           |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA   | 11       | 2.2           |
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 5        | 2.2           |
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 10       | 2.2           |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG  | 15       | 2.2           |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG  | 16       | 2.2           |
| (1,308)  | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3 | 17       | 2.2           |
| (2,935)  | 1:42:A:LYS:CB   | 1:98:A:ASP:CB  | 8        | 2.19          |
| (2,800)  | 1:126:A:LEU:CB  | 1:13:A:ILE:CB  | 19       | 2.19          |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB  | 12       | 2.19          |
| (2,171)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 11       | 2.18          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB  | 18       | 2.17          |
| (2,833)  | 1:13:A:ILE:CB   | 1:120:A:PHE:CB | 3        | 2.17          |
| (2,818)  | 1:132:A:VAL:CB  | 1:118:A:THR:CB | 14       | 2.17          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB | 4        | 2.17          |
| (2,728)  | 1:113:A:GLN:CB  | 1:116:A:ILE:CB | 12       | 2.17          |
| (2,437)  | 1:84:A:GLU:H    | 1:86:A:LEU:CB  | 5        | 2.17          |
| (2,378)  | 1:84:A:GLU:CB   | 1:45:A:TRP:CB  | 5        | 2.17          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB  | 1        | 2.17          |
| (2,171)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 9        | 2.17          |
| (1,308)  | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3 | 18       | 2.17          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 16       | 2.16          |
| (2,935)  | 1:42:A:LYS:CB   | 1:98:A:ASP:CB  | 16       | 2.16          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB  | 15       | 2.16          |
| (2,437)  | 1:84:A:GLU:H    | 1:86:A:LEU:CB  | 4        | 2.16          |
| (2,83)   | 1:44:A:TYR:CB   | 1:46:A:TYR:CB  | 10       | 2.16          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB  | 4        | 2.16          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2 | 18       | 2.16          |
| (1,537)  | 1:54:A:LYS:HB2  | 1:60:A:GLN:HB3 | 18       | 2.16          |
| (1,308)  | 1:81:A:SER:HB2  | 1:84:A:GLU:HB3 | 12       | 2.16          |
| (2,956)  | 1:9:A:TRP:CB    | 1:107:A:SER:CB | 6        | 2.15          |
| (2,833)  | 1:13:A:ILE:CB   | 1:120:A:PHE:CB | 13       | 2.15          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB   | 5        | 2.15          |
| (2,520)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB  | 4        | 2.15          |
| (2,171)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 18       | 2.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,935)  | 1:42:A:LYS:CB  | 1:98:A:ASP:CB   | 19       | 2.14          |
| (2,846)  | 1:70:A:TYR:CB  | 1:76:A:PRO:CB   | 3        | 2.14          |
| (2,761)  | 1:125:A:ILE:H  | 1:127:A:PRO:CB  | 9        | 2.14          |
| (2,376)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 4        | 2.14          |
| (2,21)   | 1:128:A:GLN:CB | 1:20:A:ARG:CB   | 5        | 2.14          |
| (1,62)   | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 6        | 2.14          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 17       | 2.13          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 17       | 2.13          |
| (2,800)  | 1:126:A:LEU:CB | 1:13:A:ILE:CB   | 7        | 2.13          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 16       | 2.13          |
| (2,514)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 19       | 2.13          |
| (2,989)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 10       | 2.12          |
| (2,956)  | 1:9:A:TRP:CB   | 1:107:A:SER:CB  | 7        | 2.12          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB   | 2        | 2.12          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB   | 11       | 2.12          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB   | 19       | 2.12          |
| (2,514)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 9        | 2.12          |
| (2,388)  | 1:65:A:PRO:CB  | 1:67:A:TRP:CB   | 4        | 2.12          |
| (2,376)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 17       | 2.12          |
| (2,35)   | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 1        | 2.12          |
| (1,1363) | 1:52:A:SER:HB2 | 1:62:A:GLN:HG2  | 3        | 2.12          |
| (2,989)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 5        | 2.11          |
| (2,778)  | 1:29:A:GLY:H   | 1:120:A:PHE:CB  | 12       | 2.11          |
| (2,582)  | 1:107:A:SER:CA | 1:9:A:TRP:CB    | 9        | 2.11          |
| (2,171)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 7        | 2.11          |
| (2,42)   | 1:80:A:ALA:CB  | 1:91:A:TRP:CB   | 4        | 2.11          |
| (2,35)   | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 12       | 2.11          |
| (1,1034) | 1:111:A:THR:HA | 1:110:A:PRO:HG3 | 7        | 2.11          |
| (2,886)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 10       | 2.1           |
| (2,860)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 10       | 2.1           |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 15       | 2.1           |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 15       | 2.1           |
| (2,6)    | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 11       | 2.1           |
| (1,1363) | 1:52:A:SER:HB2 | 1:62:A:GLN:HG2  | 2        | 2.1           |
| (1,308)  | 1:81:A:SER:HB2 | 1:84:A:GLU:HB3  | 15       | 2.1           |
| (2,833)  | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 19       | 2.09          |
| (2,818)  | 1:132:A:VAL:CB | 1:118:A:THR:CB  | 2        | 2.09          |
| (2,818)  | 1:132:A:VAL:CB | 1:118:A:THR:CB  | 8        | 2.09          |
| (2,818)  | 1:132:A:VAL:CB | 1:118:A:THR:CB  | 19       | 2.09          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 15       | 2.09          |
| (2,106)  | 1:68:A:TYR:CB  | 1:66:A:ARG:CB   | 3        | 2.09          |
| (2,106)  | 1:68:A:TYR:CB  | 1:66:A:ARG:CB   | 9        | 2.09          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,83)  | 1:44:A:TYR:CB  | 1:46:A:TYR:CB   | 13       | 2.09          |
| (1,308) | 1:81:A:SER:HB2 | 1:84:A:GLU:HB3  | 1        | 2.09          |
| (1,308) | 1:81:A:SER:HB2 | 1:84:A:GLU:HB3  | 10       | 2.09          |
| (2,833) | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 7        | 2.08          |
| (2,558) | 1:84:A:GLU:CB  | 1:86:A:LEU:CB   | 8        | 2.08          |
| (2,388) | 1:65:A:PRO:CB  | 1:67:A:TRP:CB   | 9        | 2.08          |
| (2,376) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 16       | 2.08          |
| (2,358) | 1:31:A:PRO:CB  | 1:10:A:PHE:CB   | 11       | 2.08          |
| (2,297) | 1:85:A:SER:CA  | 1:45:A:TRP:CB   | 2        | 2.08          |
| (2,226) | 1:113:A:GLN:CB | 1:9:A:TRP:CA    | 3        | 2.08          |
| (2,35)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 15       | 2.08          |
| (2,6)   | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 17       | 2.08          |
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 1        | 2.07          |
| (2,833) | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 5        | 2.07          |
| (2,641) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB   | 14       | 2.07          |
| (2,626) | 1:99:A:THR:CB  | 1:42:A:LYS:CB   | 6        | 2.07          |
| (2,558) | 1:84:A:GLU:CB  | 1:86:A:LEU:CB   | 17       | 2.07          |
| (2,520) | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 1        | 2.07          |
| (2,520) | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 18       | 2.07          |
| (2,518) | 1:94:A:ASN:CB  | 1:96:A:GLN:CB   | 3        | 2.07          |
| (2,437) | 1:84:A:GLU:H   | 1:86:A:LEU:CB   | 18       | 2.07          |
| (2,388) | 1:65:A:PRO:CB  | 1:67:A:TRP:CB   | 2        | 2.07          |
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 15       | 2.06          |
| (2,833) | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 2        | 2.06          |
| (2,558) | 1:84:A:GLU:CB  | 1:86:A:LEU:CB   | 18       | 2.06          |
| (2,406) | 1:33:A:ALA:CB  | 1:71:A:TYR:CB   | 14       | 2.06          |
| (2,6)   | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 18       | 2.06          |
| (1,62)  | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 19       | 2.06          |
| (2,839) | 1:69:A:PHE:CB  | 1:31:A:PRO:CB   | 11       | 2.05          |
| (2,833) | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 16       | 2.05          |
| (2,735) | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 8        | 2.05          |
| (2,626) | 1:99:A:THR:CB  | 1:42:A:LYS:CB   | 9        | 2.05          |
| (2,437) | 1:84:A:GLU:H   | 1:86:A:LEU:CB   | 11       | 2.05          |
| (2,423) | 1:14:A:THR:H   | 1:126:A:LEU:CB  | 11       | 2.05          |
| (2,85)  | 1:45:A:TRP:CB  | 1:91:A:TRP:CB   | 15       | 2.05          |
| (2,35)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 3        | 2.05          |
| (2,21)  | 1:128:A:GLN:CB | 1:20:A:ARG:CB   | 13       | 2.05          |
| (1,62)  | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 17       | 2.05          |
| (2,989) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 1        | 2.04          |
| (2,894) | 1:98:A:ASP:H   | 1:42:A:LYS:CB   | 11       | 2.04          |
| (2,894) | 1:98:A:ASP:H   | 1:42:A:LYS:CB   | 12       | 2.04          |
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 2        | 2.04          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 6        | 2.04          |
| (2,827) | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 3        | 2.04          |
| (2,827) | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 3        | 2.04          |
| (2,626) | 1:99:A:THR:CB  | 1:42:A:LYS:CB   | 8        | 2.04          |
| (2,520) | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 7        | 2.04          |
| (2,520) | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 11       | 2.04          |
| (2,437) | 1:84:A:GLU:H   | 1:86:A:LEU:CB   | 17       | 2.04          |
| (2,423) | 1:14:A:THR:H   | 1:126:A:LEU:CB  | 16       | 2.04          |
| (2,376) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 10       | 2.04          |
| (2,297) | 1:85:A:SER:CA  | 1:45:A:TRP:CB   | 16       | 2.04          |
| (2,6)   | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 15       | 2.04          |
| (2,989) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 12       | 2.03          |
| (2,833) | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 15       | 2.03          |
| (2,818) | 1:132:A:VAL:CB | 1:118:A:THR:CB  | 18       | 2.03          |
| (2,437) | 1:84:A:GLU:H   | 1:86:A:LEU:CB   | 9        | 2.03          |
| (2,376) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 5        | 2.03          |
| (2,35)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 2        | 2.03          |
| (1,62)  | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 16       | 2.03          |
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 11       | 2.02          |
| (2,833) | 1:13:A:ILE:CB  | 1:120:A:PHE:CB  | 9        | 2.02          |
| (2,829) | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 6        | 2.02          |
| (2,651) | 1:70:A:TYR:H   | 1:31:A:PRO:CB   | 11       | 2.02          |
| (2,641) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB   | 19       | 2.02          |
| (2,520) | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 2        | 2.02          |
| (2,437) | 1:84:A:GLU:H   | 1:86:A:LEU:CB   | 1        | 2.02          |
| (2,437) | 1:84:A:GLU:H   | 1:86:A:LEU:CB   | 10       | 2.02          |
| (2,35)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 14       | 2.02          |
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 7        | 2.01          |
| (2,818) | 1:132:A:VAL:CB | 1:118:A:THR:CB  | 7        | 2.01          |
| (2,818) | 1:132:A:VAL:CB | 1:118:A:THR:CB  | 13       | 2.01          |
| (2,808) | 1:20:A:ARG:CB  | 1:128:A:GLN:CB  | 4        | 2.01          |
| (2,792) | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 16       | 2.01          |
| (2,520) | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 12       | 2.01          |
| (1,308) | 1:81:A:SER:HB2 | 1:84:A:GLU:HB3  | 6        | 2.01          |
| (1,308) | 1:81:A:SER:HB2 | 1:84:A:GLU:HB3  | 13       | 2.01          |
| (2,989) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 15       | 2.0           |
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 13       | 2.0           |
| (2,866) | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 14       | 2.0           |
| (2,827) | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 7        | 2.0           |
| (2,827) | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 7        | 2.0           |
| (2,761) | 1:125:A:ILE:H  | 1:127:A:PRO:CB  | 17       | 2.0           |
| (2,689) | 1:106:A:SER:H  | 1:9:A:TRP:CB    | 12       | 2.0           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB  | 17       | 2.0           |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 1        | 2.0           |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 3        | 2.0           |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 9        | 2.0           |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 14       | 2.0           |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 18       | 2.0           |
| (2,833)  | 1:13:A:ILE:CB  | 1:120:A:PHE:CB | 18       | 1.99          |
| (2,818)  | 1:132:A:VAL:CB | 1:118:A:THR:CB | 11       | 1.99          |
| (2,818)  | 1:132:A:VAL:CB | 1:118:A:THR:CB | 16       | 1.99          |
| (2,808)  | 1:20:A:ARG:CB  | 1:128:A:GLN:CB | 5        | 1.99          |
| (2,761)  | 1:125:A:ILE:H  | 1:127:A:PRO:CB | 18       | 1.99          |
| (2,582)  | 1:107:A:SER:CA | 1:9:A:TRP:CB   | 13       | 1.99          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 12       | 1.99          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 12       | 1.99          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 17       | 1.99          |
| (2,226)  | 1:113:A:GLN:CB | 1:9:A:TRP:CA   | 13       | 1.99          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB  | 14       | 1.99          |
| (1,308)  | 1:81:A:SER:HB2 | 1:84:A:GLU:HB3 | 16       | 1.99          |
| (2,866)  | 1:41:A:ALA:CB  | 1:71:A:TYR:CB  | 18       | 1.98          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB  | 3        | 1.98          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 10       | 1.98          |
| (2,437)  | 1:84:A:GLU:H   | 1:86:A:LEU:CB  | 3        | 1.98          |
| (2,358)  | 1:31:A:PRO:CB  | 1:10:A:PHE:CB  | 3        | 1.98          |
| (2,297)  | 1:85:A:SER:CA  | 1:45:A:TRP:CB  | 19       | 1.98          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB  | 12       | 1.98          |
| (1,308)  | 1:81:A:SER:HB2 | 1:84:A:GLU:HB3 | 19       | 1.98          |
| (2,1019) | 1:38:A:PRO:CB  | 1:96:A:GLN:CB  | 18       | 1.97          |
| (2,989)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB | 3        | 1.97          |
| (2,866)  | 1:41:A:ALA:CB  | 1:71:A:TYR:CB  | 9        | 1.97          |
| (2,689)  | 1:106:A:SER:H  | 1:9:A:TRP:CB   | 18       | 1.97          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB  | 13       | 1.97          |
| (2,437)  | 1:84:A:GLU:H   | 1:86:A:LEU:CB  | 8        | 1.97          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 3        | 1.97          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 5        | 1.97          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 9        | 1.97          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 13       | 1.97          |
| (2,406)  | 1:33:A:ALA:CB  | 1:71:A:TYR:CB  | 5        | 1.97          |
| (2,846)  | 1:70:A:TYR:CB  | 1:76:A:PRO:CB  | 1        | 1.96          |
| (2,833)  | 1:13:A:ILE:CB  | 1:120:A:PHE:CB | 12       | 1.96          |
| (2,829)  | 1:9:A:TRP:CB   | 1:105:A:VAL:CB | 4        | 1.96          |
| (2,376)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB | 1        | 1.96          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB  | 17       | 1.96          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,6)    | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 6        | 1.96          |
| (1,62)   | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 1        | 1.96          |
| (1,62)   | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 10       | 1.96          |
| (2,989)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 2        | 1.95          |
| (2,866)  | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 10       | 1.95          |
| (2,829)  | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 3        | 1.95          |
| (2,829)  | 1:9:A:TRP:CB   | 1:105:A:VAL:CB  | 14       | 1.95          |
| (2,728)  | 1:113:A:GLN:CB | 1:116:A:ILE:CB  | 13       | 1.95          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB   | 7        | 1.95          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB  | 4        | 1.95          |
| (2,388)  | 1:65:A:PRO:CB  | 1:67:A:TRP:CB   | 8        | 1.95          |
| (2,376)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 12       | 1.95          |
| (2,239)  | 1:94:A:ASN:CB  | 1:96:A:GLN:CB   | 3        | 1.95          |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB   | 4        | 1.95          |
| (2,21)   | 1:128:A:GLN:CB | 1:20:A:ARG:CB   | 8        | 1.95          |
| (2,989)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 14       | 1.94          |
| (2,866)  | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 12       | 1.94          |
| (2,792)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 1        | 1.94          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB   | 16       | 1.94          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB   | 18       | 1.94          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 6        | 1.94          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 9        | 1.94          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB  | 2        | 1.94          |
| (2,35)   | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 13       | 1.94          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB   | 2        | 1.93          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB   | 7        | 1.93          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB   | 13       | 1.93          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB  | 10       | 1.93          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB  | 15       | 1.93          |
| (2,358)  | 1:31:A:PRO:CB  | 1:10:A:PHE:CB   | 19       | 1.93          |
| (2,866)  | 1:41:A:ALA:CB  | 1:71:A:TYR:CB   | 3        | 1.92          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 13       | 1.92          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 13       | 1.92          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB  | 14       | 1.92          |
| (2,376)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 15       | 1.92          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB   | 10       | 1.92          |
| (2,76)   | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 1        | 1.92          |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB   | 11       | 1.92          |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB   | 6        | 1.91          |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB   | 9        | 1.91          |
| (2,894)  | 1:98:A:ASP:H   | 1:42:A:LYS:CB   | 15       | 1.91          |
| (2,846)  | 1:70:A:TYR:CB  | 1:76:A:PRO:CB   | 4        | 1.91          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,846)  | 1:70:A:TYR:CB  | 1:76:A:PRO:CB  | 5        | 1.91          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB  | 12       | 1.91          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB  | 12       | 1.91          |
| (2,728)  | 1:113:A:GLN:CB | 1:116:A:ILE:CB | 19       | 1.91          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB  | 10       | 1.91          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 6        | 1.91          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 16       | 1.91          |
| (2,437)  | 1:84:A:GLU:H   | 1:86:A:LEU:CB  | 7        | 1.91          |
| (2,226)  | 1:113:A:GLN:CB | 1:9:A:TRP:CA   | 10       | 1.91          |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB  | 7        | 1.91          |
| (2,808)  | 1:20:A:ARG:CB  | 1:128:A:GLN:CB | 13       | 1.9           |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB  | 19       | 1.9           |
| (2,894)  | 1:98:A:ASP:H   | 1:42:A:LYS:CB  | 5        | 1.89          |
| (2,771)  | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 17       | 1.89          |
| (2,771)  | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 19       | 1.89          |
| (2,761)  | 1:125:A:ILE:H  | 1:127:A:PRO:CB | 11       | 1.89          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB  | 15       | 1.89          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB  | 5        | 1.89          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB  | 19       | 1.89          |
| (2,406)  | 1:33:A:ALA:CB  | 1:71:A:TYR:CB  | 13       | 1.89          |
| (2,376)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB | 3        | 1.89          |
| (1,1162) | 1:62:A:GLN:HG2 | 1:63:A:LEU:HG  | 10       | 1.89          |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB  | 8        | 1.88          |
| (2,771)  | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 16       | 1.88          |
| (2,735)  | 1:116:A:ILE:CB | 1:117:A:PRO:CB | 17       | 1.88          |
| (2,558)  | 1:84:A:GLU:CB  | 1:86:A:LEU:CB  | 5        | 1.88          |
| (2,520)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB  | 14       | 1.88          |
| (2,437)  | 1:84:A:GLU:H   | 1:86:A:LEU:CB  | 2        | 1.88          |
| (2,437)  | 1:84:A:GLU:H   | 1:86:A:LEU:CB  | 6        | 1.88          |
| (2,423)  | 1:14:A:THR:H   | 1:126:A:LEU:CB | 6        | 1.88          |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB  | 17       | 1.88          |
| (2,21)   | 1:128:A:GLN:CB | 1:20:A:ARG:CB  | 11       | 1.88          |
| (1,1363) | 1:52:A:SER:HB2 | 1:62:A:GLN:HG2 | 13       | 1.88          |
| (2,894)  | 1:98:A:ASP:H   | 1:42:A:LYS:CB  | 19       | 1.87          |
| (2,829)  | 1:9:A:TRP:CB   | 1:105:A:VAL:CB | 16       | 1.87          |
| (2,818)  | 1:132:A:VAL:CB | 1:118:A:THR:CB | 6        | 1.87          |
| (2,771)  | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 3        | 1.87          |
| (2,771)  | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 4        | 1.87          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB  | 14       | 1.87          |
| (2,376)  | 1:32:A:ILE:CB  | 1:121:A:PRO:CB | 2        | 1.87          |
| (2,297)  | 1:85:A:SER:CA  | 1:45:A:TRP:CB  | 4        | 1.87          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB  | 18       | 1.87          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 11       | 1.87          |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 5        | 1.87          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 4        | 1.86          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 4        | 1.86          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 13       | 1.86          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 4        | 1.86          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 1        | 1.86          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 14       | 1.86          |
| (2,866)  | 1:41:A:ALA:CB   | 1:71:A:TYR:CB   | 5        | 1.86          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 7        | 1.86          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 17       | 1.86          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 17       | 1.86          |
| (2,520)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 3        | 1.86          |
| (2,437)  | 1:84:A:GLU:H    | 1:86:A:LEU:CB   | 16       | 1.86          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 14       | 1.86          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 14       | 1.86          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 9        | 1.86          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 14       | 1.86          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 2        | 1.86          |
| (1,62)   | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 15       | 1.86          |
| (2,829)  | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 1        | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 2        | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 2        | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 5        | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 5        | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 6        | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 6        | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 16       | 1.85          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 16       | 1.85          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 5        | 1.85          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB  | 12       | 1.85          |
| (2,520)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 10       | 1.85          |
| (2,437)  | 1:84:A:GLU:H    | 1:86:A:LEU:CB   | 13       | 1.85          |
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 6        | 1.85          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 1        | 1.85          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG   | 19       | 1.85          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 10       | 1.84          |
| (2,829)  | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 13       | 1.84          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 10       | 1.84          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 12       | 1.84          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 15       | 1.84          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB  | 2        | 1.84          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 9        | 1.84          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 13       | 1.84          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 14       | 1.84          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 18       | 1.84          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 19       | 1.84          |
| (2,626)  | 1:99:A:THR:CB   | 1:42:A:LYS:CB  | 5        | 1.84          |
| (2,558)  | 1:84:A:GLU:CB   | 1:86:A:LEU:CB  | 13       | 1.84          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB  | 2        | 1.84          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB  | 12       | 1.84          |
| (2,80)   | 1:113:A:GLN:CB  | 1:9:A:TRP:CB   | 18       | 1.84          |
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 8        | 1.84          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG  | 4        | 1.84          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG  | 18       | 1.84          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB  | 5        | 1.83          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 16       | 1.83          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 17       | 1.83          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 19       | 1.83          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB  | 3        | 1.83          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB  | 5        | 1.83          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB  | 6        | 1.83          |
| (2,829)  | 1:9:A:TRP:CB    | 1:105:A:VAL:CB | 11       | 1.83          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 1        | 1.83          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 13       | 1.83          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 10       | 1.83          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB  | 6        | 1.83          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB  | 16       | 1.83          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB  | 6        | 1.83          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB  | 18       | 1.83          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG  | 3        | 1.83          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG  | 8        | 1.83          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2 | 9        | 1.83          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 4        | 1.82          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB  | 17       | 1.82          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB  | 18       | 1.82          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 2        | 1.82          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 11       | 1.82          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 14       | 1.82          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 3        | 1.82          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 4        | 1.82          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB | 6        | 1.82          |
| (2,626)  | 1:99:A:THR:CB   | 1:42:A:LYS:CB  | 1        | 1.82          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB   | 7        | 1.82          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,572)  | 1:89:A:VAL:CB  | 1:44:A:TYR:CB  | 7        | 1.82          |
| (2,297)  | 1:85:A:SER:CA  | 1:45:A:TRP:CB  | 11       | 1.82          |
| (2,106)  | 1:68:A:TYR:CB  | 1:66:A:ARG:CB  | 15       | 1.82          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB  | 4        | 1.82          |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB  | 15       | 1.82          |
| (2,21)   | 1:128:A:GLN:CB | 1:20:A:ARG:CB  | 2        | 1.82          |
| (1,1162) | 1:62:A:GLN:HG2 | 1:63:A:LEU:HG  | 14       | 1.82          |
| (1,1162) | 1:62:A:GLN:HG2 | 1:63:A:LEU:HG  | 17       | 1.82          |
| (2,1113) | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 3        | 1.81          |
| (2,956)  | 1:9:A:TRP:CB   | 1:107:A:SER:CB | 5        | 1.81          |
| (2,833)  | 1:13:A:ILE:CB  | 1:120:A:PHE:CB | 11       | 1.81          |
| (2,735)  | 1:116:A:ILE:CB | 1:117:A:PRO:CB | 1        | 1.81          |
| (2,651)  | 1:70:A:TYR:H   | 1:31:A:PRO:CB  | 3        | 1.81          |
| (2,56)   | 1:20:A:ARG:CB  | 1:128:A:GLN:CB | 4        | 1.81          |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB  | 14       | 1.81          |
| (2,6)    | 1:48:A:HIS:CB  | 1:68:A:TYR:CB  | 7        | 1.81          |
| (2,1113) | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 5        | 1.8           |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB  | 14       | 1.8           |
| (2,894)  | 1:98:A:ASP:H   | 1:42:A:LYS:CB  | 2        | 1.8           |
| (2,894)  | 1:98:A:ASP:H   | 1:42:A:LYS:CB  | 7        | 1.8           |
| (2,808)  | 1:20:A:ARG:CB  | 1:128:A:GLN:CB | 8        | 1.8           |
| (2,761)  | 1:125:A:ILE:H  | 1:127:A:PRO:CB | 13       | 1.8           |
| (2,761)  | 1:125:A:ILE:H  | 1:127:A:PRO:CB | 14       | 1.8           |
| (2,735)  | 1:116:A:ILE:CB | 1:117:A:PRO:CB | 11       | 1.8           |
| (2,735)  | 1:116:A:ILE:CB | 1:117:A:PRO:CB | 15       | 1.8           |
| (2,735)  | 1:116:A:ILE:CB | 1:117:A:PRO:CB | 16       | 1.8           |
| (2,572)  | 1:89:A:VAL:CB  | 1:44:A:TYR:CB  | 13       | 1.8           |
| (2,106)  | 1:68:A:TYR:CB  | 1:66:A:ARG:CB  | 16       | 1.8           |
| (2,35)   | 1:32:A:ILE:CB  | 1:121:A:PRO:CB | 11       | 1.8           |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB  | 3        | 1.8           |
| (1,1363) | 1:52:A:SER:HB2 | 1:62:A:GLN:HG2 | 17       | 1.8           |
| (2,1113) | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 10       | 1.79          |
| (2,1113) | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 12       | 1.79          |
| (2,1113) | 1:122:A:PRO:CB | 1:121:A:PRO:CB | 15       | 1.79          |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB  | 5        | 1.79          |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB  | 7        | 1.79          |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB  | 18       | 1.79          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB  | 18       | 1.79          |
| (2,827)  | 1:46:A:TYR:CB  | 1:76:A:PRO:CB  | 18       | 1.79          |
| (2,735)  | 1:116:A:ILE:CB | 1:117:A:PRO:CB | 7        | 1.79          |
| (2,626)  | 1:99:A:THR:CB  | 1:42:A:LYS:CB  | 4        | 1.79          |
| (2,572)  | 1:89:A:VAL:CB  | 1:44:A:TYR:CB  | 2        | 1.79          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 18       | 1.79          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 3        | 1.79          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 10       | 1.79          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 9        | 1.79          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 5        | 1.79          |
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 9        | 1.79          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 2        | 1.79          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 8        | 1.79          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 2        | 1.79          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 9        | 1.79          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 10       | 1.79          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 5        | 1.79          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 1        | 1.78          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 13       | 1.78          |
| (2,866)  | 1:41:A:ALA:CB   | 1:71:A:TYR:CB   | 8        | 1.78          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 19       | 1.78          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 19       | 1.78          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 3        | 1.78          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 12       | 1.78          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 18       | 1.78          |
| (2,626)  | 1:99:A:THR:CB   | 1:42:A:LYS:CB   | 12       | 1.78          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 3        | 1.78          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 4        | 1.78          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 13       | 1.78          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 4        | 1.78          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG   | 13       | 1.78          |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 9        | 1.78          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 2        | 1.77          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 11       | 1.77          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 15       | 1.77          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 6        | 1.77          |
| (2,866)  | 1:41:A:ALA:CB   | 1:71:A:TYR:CB   | 17       | 1.77          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 11       | 1.77          |
| (2,735)  | 1:116:A:ILE:CB  | 1:117:A:PRO:CB  | 5        | 1.77          |
| (2,520)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 17       | 1.77          |
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 18       | 1.77          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 10       | 1.77          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 6        | 1.77          |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 2        | 1.77          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 5        | 1.77          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 17       | 1.77          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 19       | 1.77          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 19       | 1.77          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 14       | 1.76          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 8        | 1.76          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 4        | 1.76          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 19       | 1.76          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 1        | 1.76          |
| (2,514)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 13       | 1.76          |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 1        | 1.76          |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 6        | 1.76          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 12       | 1.76          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 17       | 1.76          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 19       | 1.76          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 5        | 1.76          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 14       | 1.76          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 9        | 1.76          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 2        | 1.75          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 10       | 1.75          |
| (2,818)  | 1:132:A:VAL:CB  | 1:118:A:THR:CB  | 1        | 1.75          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 6        | 1.75          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 11       | 1.75          |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 11       | 1.75          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 2        | 1.75          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 6        | 1.75          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 1        | 1.75          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 9        | 1.75          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 3        | 1.75          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 6        | 1.75          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 10       | 1.74          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 10       | 1.74          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 6        | 1.74          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 8        | 1.74          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 18       | 1.74          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 2        | 1.74          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 15       | 1.74          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 9        | 1.74          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 14       | 1.73          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 14       | 1.73          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 12       | 1.73          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 14       | 1.73          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 11       | 1.73          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 8        | 1.73          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 19       | 1.73          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,35)   | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 7        | 1.73          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 12       | 1.73          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 16       | 1.73          |
| (1,975)  | 1:96:A:GLN:H    | 1:94:A:ASN:HA   | 3        | 1.73          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 12       | 1.73          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 16       | 1.72          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 11       | 1.72          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 4        | 1.72          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 1        | 1.72          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 14       | 1.72          |
| (2,423)  | 1:14:A:THR:H    | 1:126:A:LEU:CB  | 8        | 1.72          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 18       | 1.72          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 11       | 1.72          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 12       | 1.72          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 3        | 1.72          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 13       | 1.72          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 7        | 1.72          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 14       | 1.72          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 18       | 1.72          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 10       | 1.71          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 13       | 1.71          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 9        | 1.71          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 17       | 1.71          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 11       | 1.71          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 12       | 1.71          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 8        | 1.71          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 8        | 1.71          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 10       | 1.71          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 11       | 1.71          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 12       | 1.71          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 15       | 1.7           |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 17       | 1.7           |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 14       | 1.7           |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 6        | 1.7           |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 10       | 1.7           |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 15       | 1.7           |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 16       | 1.7           |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 7        | 1.7           |
| (2,626)  | 1:99:A:THR:CB   | 1:42:A:LYS:CB   | 11       | 1.7           |
| (2,626)  | 1:99:A:THR:CB   | 1:42:A:LYS:CB   | 19       | 1.7           |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 8        | 1.7           |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 14       | 1.7           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 5        | 1.7           |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 13       | 1.7           |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 3        | 1.7           |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 5        | 1.7           |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 12       | 1.7           |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 19       | 1.7           |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 2        | 1.7           |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 4        | 1.7           |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 5        | 1.7           |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 9        | 1.7           |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 17       | 1.7           |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 14       | 1.7           |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 13       | 1.7           |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 18       | 1.69          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 10       | 1.69          |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 2        | 1.69          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 14       | 1.69          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 4        | 1.69          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 10       | 1.69          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 13       | 1.69          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 9        | 1.69          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 10       | 1.69          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 16       | 1.69          |
| (1,537)  | 1:54:A:LYS:HB2  | 1:60:A:GLN:HB3  | 17       | 1.69          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 1        | 1.69          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 13       | 1.69          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 16       | 1.69          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 2        | 1.69          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 4        | 1.68          |
| (2,827)  | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 4        | 1.68          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 18       | 1.68          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 13       | 1.68          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 9        | 1.68          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 10       | 1.68          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 8        | 1.68          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 8        | 1.68          |
| (2,520)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 8        | 1.68          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 8        | 1.68          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 6        | 1.68          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 8        | 1.68          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 3        | 1.68          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 15       | 1.68          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 16       | 1.68          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 16       | 1.68          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 4        | 1.68          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 8        | 1.68          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 12       | 1.68          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 5        | 1.67          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 6        | 1.67          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 4        | 1.67          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 5        | 1.67          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 7        | 1.67          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 5        | 1.67          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 1        | 1.67          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 13       | 1.67          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 2        | 1.67          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 6        | 1.67          |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 13       | 1.67          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 18       | 1.67          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 3        | 1.67          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 14       | 1.67          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 9        | 1.67          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 9        | 1.67          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 1        | 1.66          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 1        | 1.66          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 8        | 1.66          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 1        | 1.66          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 8        | 1.66          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 5        | 1.66          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 5        | 1.66          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG   | 2        | 1.66          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 5        | 1.66          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 4        | 1.66          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 7        | 1.66          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 18       | 1.66          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 9        | 1.65          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 13       | 1.65          |
| (2,989)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 7        | 1.65          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 9        | 1.65          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 4        | 1.65          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 11       | 1.65          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 4        | 1.65          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 4        | 1.65          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 9        | 1.65          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 15       | 1.65          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 2        | 1.65          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 11       | 1.65          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 12       | 1.65          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 15       | 1.65          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 17       | 1.65          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 7        | 1.64          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 18       | 1.64          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 13       | 1.64          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 16       | 1.64          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 16       | 1.64          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 13       | 1.64          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 2        | 1.64          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 13       | 1.64          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 11       | 1.64          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 6        | 1.64          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 5        | 1.64          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 7        | 1.64          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 6        | 1.64          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 18       | 1.64          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 6        | 1.64          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 13       | 1.64          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 3        | 1.64          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 7        | 1.64          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 8        | 1.63          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 4        | 1.63          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 5        | 1.63          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 7        | 1.63          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 18       | 1.63          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 9        | 1.63          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 18       | 1.63          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 18       | 1.63          |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 14       | 1.63          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 11       | 1.63          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 14       | 1.63          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 15       | 1.63          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 16       | 1.63          |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 12       | 1.63          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 9        | 1.62          |
| (2,1018) | 1:50:A:ARG:CB   | 1:66:A:ARG:CB   | 13       | 1.62          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 10       | 1.62          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 9        | 1.62          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB  | 17       | 1.62          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB | 6        | 1.62          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB  | 5        | 1.62          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB  | 18       | 1.62          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB  | 18       | 1.62          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB  | 8        | 1.62          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB  | 3        | 1.62          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB  | 12       | 1.62          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB  | 19       | 1.62          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB  | 18       | 1.62          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2 | 8        | 1.62          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2 | 6        | 1.62          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB | 7        | 1.61          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB | 7        | 1.61          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB  | 15       | 1.61          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB  | 18       | 1.61          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB | 7        | 1.61          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 6        | 1.61          |
| (2,771)  | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 9        | 1.61          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB | 2        | 1.61          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB   | 15       | 1.61          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB  | 15       | 1.61          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB  | 19       | 1.61          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB | 16       | 1.61          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB | 18       | 1.61          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB  | 1        | 1.61          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB  | 14       | 1.61          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2 | 1        | 1.61          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2 | 6        | 1.61          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2 | 8        | 1.61          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB | 8        | 1.6           |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB  | 14       | 1.6           |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB  | 17       | 1.6           |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB  | 19       | 1.6           |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB  | 12       | 1.6           |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB  | 15       | 1.6           |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB  | 15       | 1.6           |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB  | 5        | 1.6           |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB  | 7        | 1.6           |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB  | 16       | 1.6           |
| (2,237)  | 1:24:A:PHE:H    | 1:90:A:PHE:CB  | 2        | 1.6           |
| (2,111)  | 1:9:A:TRP:CA    | 1:71:A:TYR:CB  | 17       | 1.6           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 8        | 1.6           |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 4        | 1.6           |
| (1,1034) | 1:111:A:THR:HA  | 1:110:A:PRO:HG3 | 1        | 1.6           |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 6        | 1.6           |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 5        | 1.6           |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 6        | 1.59          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 13       | 1.59          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 18       | 1.59          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 1        | 1.59          |
| (2,572)  | 1:89:A:VAL:CB   | 1:44:A:TYR:CB   | 17       | 1.59          |
| (2,514)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 17       | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 2        | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 4        | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 6        | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 8        | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 10       | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 11       | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 13       | 1.59          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 15       | 1.59          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 3        | 1.59          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 4        | 1.59          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 5        | 1.59          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 18       | 1.58          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 14       | 1.58          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 11       | 1.58          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 1        | 1.58          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 16       | 1.58          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 15       | 1.58          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 3        | 1.58          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 12       | 1.58          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 16       | 1.58          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 3        | 1.58          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 10       | 1.58          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 10       | 1.58          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 12       | 1.58          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 12       | 1.58          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 9        | 1.58          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 11       | 1.58          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 2        | 1.58          |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 11       | 1.58          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 7        | 1.57          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 10       | 1.57          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,829)  | 1:9:A:TRP:CB    | 1:105:A:VAL:CB  | 19       | 1.57          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 7        | 1.57          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 4        | 1.57          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 10       | 1.57          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 5        | 1.57          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 14       | 1.57          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 13       | 1.57          |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 1        | 1.57          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 1        | 1.57          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 6        | 1.56          |
| (2,1113) | 1:122:A:PRO:CB  | 1:121:A:PRO:CB  | 9        | 1.56          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 2        | 1.56          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 5        | 1.56          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 6        | 1.56          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 7        | 1.56          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 7        | 1.56          |
| (2,423)  | 1:14:A:THR:H    | 1:126:A:LEU:CB  | 1        | 1.56          |
| (2,376)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 7        | 1.56          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 17       | 1.56          |
| (2,348)  | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 18       | 1.56          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 8        | 1.56          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 9        | 1.56          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 14       | 1.56          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 19       | 1.56          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 13       | 1.56          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 11       | 1.56          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 13       | 1.55          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 16       | 1.55          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 16       | 1.55          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 7        | 1.55          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 14       | 1.55          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 14       | 1.55          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 17       | 1.55          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 11       | 1.55          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 15       | 1.55          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 1        | 1.55          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 5        | 1.55          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 18       | 1.55          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 15       | 1.54          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 19       | 1.54          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 10       | 1.54          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 9        | 1.54          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 10       | 1.54          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 17       | 1.54          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 2        | 1.54          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 18       | 1.54          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 18       | 1.54          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 19       | 1.54          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 4        | 1.54          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 7        | 1.54          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 9        | 1.54          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 6        | 1.54          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 10       | 1.54          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 4        | 1.54          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 3        | 1.53          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 11       | 1.53          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 15       | 1.53          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 18       | 1.53          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 19       | 1.53          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 9        | 1.53          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 9        | 1.53          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 12       | 1.53          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 15       | 1.53          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 15       | 1.53          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 15       | 1.53          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 1        | 1.53          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 8        | 1.53          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 13       | 1.53          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 11       | 1.53          |
| (2,54)   | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 1        | 1.53          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 9        | 1.53          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 18       | 1.53          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 7        | 1.53          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 14       | 1.53          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 18       | 1.53          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 2        | 1.52          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 13       | 1.52          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 2        | 1.52          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 2        | 1.52          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 3        | 1.52          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 8        | 1.52          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 15       | 1.52          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 4        | 1.52          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 17       | 1.52          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 9        | 1.52          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 11       | 1.52          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2  | 11       | 1.52          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 4        | 1.52          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 16       | 1.52          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 14       | 1.52          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 4        | 1.51          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 5        | 1.51          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 19       | 1.51          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 19       | 1.51          |
| (2,956)  | 1:9:A:TRP:CB    | 1:107:A:SER:CB  | 8        | 1.51          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 7        | 1.51          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 12       | 1.51          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 12       | 1.51          |
| (2,761)  | 1:125:A:ILE:H   | 1:127:A:PRO:CB  | 7        | 1.51          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 12       | 1.51          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 18       | 1.51          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 2        | 1.51          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 13       | 1.51          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 13       | 1.51          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 13       | 1.51          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 5        | 1.51          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 5        | 1.51          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 15       | 1.51          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 19       | 1.51          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 12       | 1.51          |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 1        | 1.5           |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 16       | 1.5           |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 17       | 1.5           |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 14       | 1.5           |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 3        | 1.5           |
| (2,728)  | 1:113:A:GLN:CB  | 1:116:A:ILE:CB  | 16       | 1.5           |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 1        | 1.5           |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 1        | 1.5           |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 11       | 1.5           |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 11       | 1.5           |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 12       | 1.5           |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 12       | 1.5           |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 7        | 1.5           |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 7        | 1.5           |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 14       | 1.5           |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB   | 16       | 1.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 13       | 1.5           |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 13       | 1.5           |
| (2,1110) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 12       | 1.49          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB   | 19       | 1.49          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 10       | 1.49          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 13       | 1.49          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 14       | 1.49          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 9        | 1.49          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 7        | 1.49          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 17       | 1.49          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 5        | 1.49          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 14       | 1.49          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 14       | 1.49          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 9        | 1.49          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 19       | 1.49          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 19       | 1.49          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 19       | 1.49          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 9        | 1.49          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 9        | 1.49          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 17       | 1.49          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 17       | 1.49          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 18       | 1.49          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 5        | 1.49          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 17       | 1.49          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 15       | 1.49          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 8        | 1.49          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 9        | 1.49          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 13       | 1.49          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 7        | 1.49          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 2        | 1.48          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 8        | 1.48          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 12       | 1.48          |
| (2,846)  | 1:70:A:TYR:CB   | 1:76:A:PRO:CB   | 12       | 1.48          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 8        | 1.48          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 14       | 1.48          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 2        | 1.48          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 14       | 1.48          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 14       | 1.48          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 3        | 1.48          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 2        | 1.48          |
| (2,1018) | 1:50:A:ARG:CB   | 1:66:A:ARG:CB   | 8        | 1.47          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 1        | 1.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 2        | 1.47          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 2        | 1.47          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 18       | 1.47          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 3        | 1.47          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 14       | 1.47          |
| (2,514)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 3        | 1.47          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 3        | 1.47          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 3        | 1.47          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 6        | 1.47          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 2        | 1.47          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 9        | 1.46          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 19       | 1.46          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 9        | 1.46          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 11       | 1.46          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 5        | 1.46          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 2        | 1.46          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 6        | 1.46          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 3        | 1.46          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 2        | 1.46          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 16       | 1.46          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 11       | 1.46          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 11       | 1.46          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 18       | 1.46          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 14       | 1.46          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 1        | 1.46          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 2        | 1.46          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 9        | 1.46          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 6        | 1.46          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 10       | 1.46          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 18       | 1.46          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 8        | 1.45          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 2        | 1.45          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 18       | 1.45          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 6        | 1.45          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 6        | 1.45          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 1        | 1.45          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 1        | 1.45          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 2        | 1.45          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 2        | 1.45          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 9        | 1.45          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 14       | 1.45          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 15       | 1.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 1        | 1.45          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 7        | 1.45          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 10       | 1.45          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 5        | 1.44          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 11       | 1.44          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 14       | 1.44          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 14       | 1.44          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 14       | 1.44          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 8        | 1.44          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 16       | 1.44          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 12       | 1.44          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 18       | 1.44          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 9        | 1.44          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 16       | 1.44          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 16       | 1.44          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 6        | 1.44          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 6        | 1.44          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 8        | 1.44          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 8        | 1.44          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 13       | 1.44          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 13       | 1.44          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 9        | 1.44          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB   | 10       | 1.44          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 13       | 1.44          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 14       | 1.44          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 1        | 1.44          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2  | 19       | 1.44          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 3        | 1.43          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 9        | 1.43          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 17       | 1.43          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 10       | 1.43          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 19       | 1.43          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 2        | 1.43          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 7        | 1.43          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 10       | 1.43          |
| (2,646)  | 1:105:A:VAL:CB  | 1:103:A:SER:CB  | 17       | 1.43          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 3        | 1.43          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 3        | 1.43          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 5        | 1.43          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 5        | 1.43          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 13       | 1.43          |
| (2,423)  | 1:14:A:THR:H    | 1:126:A:LEU:CB  | 7        | 1.43          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB  | 1        | 1.43          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB  | 12       | 1.43          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB  | 11       | 1.43          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB  | 4        | 1.43          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB  | 6        | 1.43          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB  | 15       | 1.43          |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3 | 3        | 1.43          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB  | 11       | 1.42          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB  | 2        | 1.42          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB  | 11       | 1.42          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB  | 8        | 1.42          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB  | 9        | 1.42          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB  | 9        | 1.42          |
| (2,514)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB   | 8        | 1.42          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB  | 10       | 1.42          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB  | 10       | 1.42          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB  | 17       | 1.42          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB  | 11       | 1.42          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB  | 9        | 1.42          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB  | 1        | 1.42          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB | 6        | 1.42          |
| (2,25)   | 1:72:A:LEU:CB   | 1:82:A:TYR:CB  | 13       | 1.42          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2 | 16       | 1.42          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2 | 17       | 1.42          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3 | 15       | 1.42          |
| (1,195)  | 1:103:A:SER:H   | 1:72:A:LEU:HB2 | 13       | 1.42          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 16       | 1.41          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB  | 14       | 1.41          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB  | 15       | 1.41          |
| (2,442)  | 1:37:A:PRO:CB   | 1:36:A:VAL:CB  | 18       | 1.41          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB | 2        | 1.41          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB  | 11       | 1.41          |
| (2,297)  | 1:85:A:SER:CA   | 1:45:A:TRP:CB  | 18       | 1.41          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 16       | 1.41          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB  | 16       | 1.41          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2 | 3        | 1.41          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3 | 11       | 1.41          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1  | 4        | 1.41          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB  | 13       | 1.4           |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB  | 5        | 1.4           |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB  | 16       | 1.4           |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB   | 7        | 1.4           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 11       | 1.4           |
| (2,403)  | 1:105:A:VAL:H    | 1:74:A:THR:CB   | 14       | 1.4           |
| (2,387)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 14       | 1.4           |
| (2,297)  | 1:85:A:SER:CA    | 1:45:A:TRP:CB   | 17       | 1.4           |
| (2,182)  | 1:18:A:LYS:CB    | 1:64:A:LEU:CB   | 12       | 1.4           |
| (2,76)   | 1:46:A:TYR:CB    | 1:76:A:PRO:CB   | 17       | 1.4           |
| (1,1096) | 1:119:A:ARG:HG3  | 1:117:A:PRO:HG3 | 4        | 1.4           |
| (1,844)  | 1:20:A:ARG:HB3   | 1:17:A:GLN:HE21 | 17       | 1.4           |
| (2,939)  | 1:82:A:TYR:H     | 1:72:A:LEU:CB   | 2        | 1.39          |
| (2,938)  | 1:44:A:TYR:CB    | 1:72:A:LEU:CB   | 3        | 1.39          |
| (2,565)  | 1:66:A:ARG:H     | 1:67:A:TRP:CB   | 10       | 1.39          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 1        | 1.39          |
| (2,415)  | 1:44:A:TYR:H     | 1:92:A:VAL:CB   | 15       | 1.39          |
| (2,387)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 15       | 1.39          |
| (2,182)  | 1:18:A:LYS:CB    | 1:64:A:LEU:CB   | 16       | 1.39          |
| (2,56)   | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 18       | 1.39          |
| (1,844)  | 1:20:A:ARG:HB3   | 1:17:A:GLN:HE21 | 2        | 1.39          |
| (1,245)  | 1:113:A:GLN:HE21 | 1:9:A:TRP:HA    | 17       | 1.39          |
| (2,999)  | 1:130:A:TYR:H    | 1:13:A:ILE:CB   | 12       | 1.38          |
| (2,999)  | 1:130:A:TYR:H    | 1:13:A:ILE:CB   | 16       | 1.38          |
| (2,938)  | 1:44:A:TYR:CB    | 1:72:A:LEU:CB   | 8        | 1.38          |
| (2,854)  | 1:14:A:THR:CA    | 1:66:A:ARG:CB   | 19       | 1.38          |
| (2,808)  | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 9        | 1.38          |
| (2,565)  | 1:66:A:ARG:H     | 1:67:A:TRP:CB   | 15       | 1.38          |
| (2,534)  | 1:72:A:LEU:CA    | 1:44:A:TYR:CB   | 7        | 1.38          |
| (2,534)  | 1:72:A:LEU:CA    | 1:44:A:TYR:CB   | 7        | 1.38          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 2        | 1.38          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 5        | 1.38          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 13       | 1.38          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 15       | 1.38          |
| (2,387)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 5        | 1.38          |
| (2,387)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 19       | 1.38          |
| (2,56)   | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 16       | 1.38          |
| (1,1096) | 1:119:A:ARG:HG3  | 1:117:A:PRO:HG3 | 3        | 1.38          |
| (1,844)  | 1:20:A:ARG:HB3   | 1:17:A:GLN:HE21 | 5        | 1.38          |
| (1,844)  | 1:20:A:ARG:HB3   | 1:17:A:GLN:HE21 | 12       | 1.38          |
| (2,792)  | 1:108:A:ARG:H    | 1:9:A:TRP:CB    | 15       | 1.37          |
| (2,751)  | 1:118:A:THR:CB   | 1:31:A:PRO:CB   | 10       | 1.37          |
| (2,641)  | 1:47:A:ARG:CB    | 1:67:A:TRP:CB   | 15       | 1.37          |
| (2,584)  | 1:108:A:ARG:CB   | 1:9:A:TRP:CB    | 8        | 1.37          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 3        | 1.37          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 6        | 1.37          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,442)  | 1:37:A:PRO:CB  | 1:36:A:VAL:CB   | 7        | 1.37          |
| (2,442)  | 1:37:A:PRO:CB  | 1:36:A:VAL:CB   | 9        | 1.37          |
| (2,442)  | 1:37:A:PRO:CB  | 1:36:A:VAL:CB   | 12       | 1.37          |
| (2,442)  | 1:37:A:PRO:CB  | 1:36:A:VAL:CB   | 17       | 1.37          |
| (2,387)  | 1:94:A:ASN:CB  | 1:96:A:GLN:CB   | 9        | 1.37          |
| (2,387)  | 1:94:A:ASN:CB  | 1:96:A:GLN:CB   | 18       | 1.37          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB   | 8        | 1.37          |
| (2,76)   | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 15       | 1.37          |
| (2,56)   | 1:20:A:ARG:CB  | 1:128:A:GLN:CB  | 12       | 1.37          |
| (2,1019) | 1:38:A:PRO:CB  | 1:96:A:GLN:CB   | 6        | 1.36          |
| (2,975)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB   | 4        | 1.36          |
| (2,939)  | 1:82:A:TYR:H   | 1:72:A:LEU:CB   | 11       | 1.36          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 17       | 1.36          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 19       | 1.36          |
| (2,904)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 2        | 1.36          |
| (2,593)  | 1:16:A:PHE:H   | 1:64:A:LEU:CB   | 4        | 1.36          |
| (2,579)  | 1:4:A:ILE:H    | 1:5:A:PRO:CB    | 3        | 1.36          |
| (2,442)  | 1:37:A:PRO:CB  | 1:36:A:VAL:CB   | 10       | 1.36          |
| (2,442)  | 1:37:A:PRO:CB  | 1:36:A:VAL:CB   | 14       | 1.36          |
| (2,387)  | 1:94:A:ASN:CB  | 1:96:A:GLN:CB   | 8        | 1.36          |
| (2,332)  | 1:4:A:ILE:H    | 1:5:A:PRO:CB    | 3        | 1.36          |
| (2,216)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB   | 4        | 1.36          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB   | 8        | 1.36          |
| (2,85)   | 1:45:A:TRP:CB  | 1:91:A:TRP:CB   | 16       | 1.36          |
| (2,21)   | 1:128:A:GLN:CB | 1:20:A:ARG:CB   | 17       | 1.36          |
| (2,5)    | 1:44:A:TYR:H   | 1:91:A:TRP:CB   | 15       | 1.36          |
| (1,1154) | 1:11:A:SER:HA  | 1:136:A:GLY:HA3 | 17       | 1.36          |
| (2,1019) | 1:38:A:PRO:CB  | 1:96:A:GLN:CB   | 10       | 1.35          |
| (2,975)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB   | 1        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 1        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 2        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 3        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 4        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 6        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 8        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 9        | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 11       | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 12       | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 13       | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 14       | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 16       | 1.35          |
| (2,905)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 18       | 1.35          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB  | 8        | 1.35          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB  | 14       | 1.35          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB | 11       | 1.35          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB | 19       | 1.35          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB  | 12       | 1.35          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB  | 11       | 1.35          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB   | 3        | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 4        | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 6        | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 7        | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 8        | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 11       | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 12       | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 13       | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 17       | 1.35          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 18       | 1.35          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB  | 15       | 1.35          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB  | 2        | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 4        | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 6        | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 7        | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 8        | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 11       | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 12       | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 13       | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 17       | 1.35          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB   | 18       | 1.35          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 1        | 1.35          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB  | 6        | 1.35          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB  | 2        | 1.35          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2 | 5        | 1.35          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1  | 17       | 1.35          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3 | 7        | 1.35          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB  | 3        | 1.34          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB  | 4        | 1.34          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 11       | 1.34          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 15       | 1.34          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 2        | 1.34          |
| (2,905)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB | 5        | 1.34          |
| (2,905)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB | 7        | 1.34          |
| (2,905)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB | 10       | 1.34          |
| (2,905)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB | 15       | 1.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 4        | 1.34          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 6        | 1.34          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 13       | 1.34          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 17       | 1.34          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 19       | 1.34          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 5        | 1.34          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 3        | 1.34          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 1        | 1.34          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 6        | 1.34          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 5        | 1.34          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 14       | 1.34          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 15       | 1.34          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 16       | 1.34          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 19       | 1.34          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 14       | 1.34          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 17       | 1.34          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 5        | 1.34          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 14       | 1.34          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 15       | 1.34          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 16       | 1.34          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 19       | 1.34          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 11       | 1.34          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 15       | 1.34          |
| (2,21)   | 1:128:A:GLN:CB  | 1:20:A:ARG:CB   | 19       | 1.34          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 3        | 1.34          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 12       | 1.34          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 16       | 1.34          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 10       | 1.34          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 16       | 1.33          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 18       | 1.33          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 4        | 1.33          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 8        | 1.33          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 16       | 1.33          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 3        | 1.33          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 9        | 1.33          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 10       | 1.33          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 11       | 1.33          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 4        | 1.33          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 9        | 1.33          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB   | 15       | 1.33          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 10       | 1.33          |
| (2,442)  | 1:37:A:PRO:CB   | 1:36:A:VAL:CB   | 8        | 1.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 7        | 1.33          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 10       | 1.33          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 12       | 1.33          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 10       | 1.33          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB   | 17       | 1.33          |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 8        | 1.33          |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 13       | 1.33          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 3        | 1.33          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 14       | 1.32          |
| (2,956)  | 1:9:A:TRP:CB    | 1:107:A:SER:CB  | 19       | 1.32          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 5        | 1.32          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 12       | 1.32          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 14       | 1.32          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 19       | 1.32          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 4        | 1.32          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 6        | 1.32          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 13       | 1.32          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 17       | 1.32          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 19       | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 5        | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 7        | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 8        | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 12       | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 14       | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 15       | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 16       | 1.32          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 18       | 1.32          |
| (2,894)  | 1:98:A:ASP:H    | 1:42:A:LYS:CB   | 3        | 1.32          |
| (2,680)  | 1:94:A:ASN:H    | 1:99:A:THR:CB   | 1        | 1.32          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 11       | 1.32          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 15       | 1.32          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 13       | 1.32          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 14       | 1.32          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 3        | 1.32          |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 7        | 1.32          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 3        | 1.32          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 16       | 1.32          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 15       | 1.32          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 19       | 1.32          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 2        | 1.31          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 3        | 1.31          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 6        | 1.31          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 7        | 1.31          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 9        | 1.31          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 10       | 1.31          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 13       | 1.31          |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 17       | 1.31          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 3        | 1.31          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 7        | 1.31          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 8        | 1.31          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 9        | 1.31          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 10       | 1.31          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 11       | 1.31          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 12       | 1.31          |
| (2,904)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 1        | 1.31          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB  | 8        | 1.31          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB  | 8        | 1.31          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB  | 8        | 1.31          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB   | 14       | 1.31          |
| (2,751)  | 1:118:A:THR:CB  | 1:31:A:PRO:CB  | 14       | 1.31          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB | 12       | 1.31          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB | 12       | 1.31          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB   | 17       | 1.31          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB  | 12       | 1.31          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB  | 3        | 1.31          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB   | 2        | 1.31          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3 | 15       | 1.31          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2 | 12       | 1.31          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3 | 19       | 1.31          |
| (2,1082) | 1:100:A:SER:H   | 1:42:A:LYS:CB  | 1        | 1.3           |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB  | 1        | 1.3           |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 5        | 1.3           |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 10       | 1.3           |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB  | 13       | 1.3           |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 1        | 1.3           |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 11       | 1.3           |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 15       | 1.3           |
| (2,953)  | 1:36:A:VAL:CA   | 1:37:A:PRO:CB  | 18       | 1.3           |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 5        | 1.3           |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 14       | 1.3           |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 15       | 1.3           |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 16       | 1.3           |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA   | 18       | 1.3           |
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB  | 10       | 1.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 11       | 1.3           |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 10       | 1.3           |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 3        | 1.3           |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 5        | 1.3           |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 4        | 1.3           |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 16       | 1.3           |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 5        | 1.3           |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 10       | 1.3           |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 13       | 1.3           |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 3        | 1.3           |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 17       | 1.3           |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 19       | 1.3           |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG   | 12       | 1.3           |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 2        | 1.3           |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 7        | 1.29          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 14       | 1.29          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 3        | 1.29          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 10       | 1.29          |
| (2,952)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 1        | 1.29          |
| (2,939)  | 1:82:A:TYR:H    | 1:72:A:LEU:CB   | 4        | 1.29          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 10       | 1.29          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 12       | 1.29          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 14       | 1.29          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 2        | 1.29          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 2        | 1.29          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 6        | 1.29          |
| (2,534)  | 1:72:A:LEU:CA   | 1:44:A:TYR:CB   | 6        | 1.29          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 4        | 1.29          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 5        | 1.29          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 14       | 1.29          |
| (2,387)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 6        | 1.29          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 7        | 1.29          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 7        | 1.29          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 14       | 1.29          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 18       | 1.29          |
| (1,372)  | 1:97:A:ALA:H    | 1:94:A:ASN:HB2  | 3        | 1.29          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3  | 18       | 1.29          |
| (2,1149) | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 10       | 1.28          |
| (2,1148) | 1:64:A:LEU:CB   | 1:18:A:LYS:CB   | 10       | 1.28          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 17       | 1.28          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 9        | 1.28          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 15       | 1.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 1        | 1.28          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 1        | 1.28          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3  | 9        | 1.28          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB  | 4        | 1.27          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 3        | 1.27          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 7        | 1.27          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 11       | 1.27          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 11       | 1.27          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 6        | 1.27          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 6        | 1.27          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 13       | 1.27          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 1        | 1.27          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 3        | 1.27          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 19       | 1.27          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 7        | 1.27          |
| (1,1269) | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 11       | 1.27          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 4        | 1.27          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 13       | 1.27          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 4        | 1.27          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 19       | 1.27          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 13       | 1.26          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 11       | 1.26          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 13       | 1.26          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 10       | 1.26          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 2        | 1.26          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 6        | 1.26          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 4        | 1.26          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 19       | 1.26          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 13       | 1.26          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 19       | 1.26          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 9        | 1.26          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 2        | 1.26          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3  | 3        | 1.26          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 7        | 1.25          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 7        | 1.25          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 4        | 1.25          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 15       | 1.25          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 2        | 1.25          |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 16       | 1.25          |
| (2,423)  | 1:14:A:THR:H    | 1:126:A:LEU:CB  | 19       | 1.25          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 2        | 1.25          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 12       | 1.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 17       | 1.25          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 19       | 1.25          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 1        | 1.25          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 5        | 1.25          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 13       | 1.25          |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 13       | 1.24          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 17       | 1.24          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 6        | 1.24          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 5        | 1.24          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 7        | 1.24          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 4        | 1.24          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 3        | 1.24          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 10       | 1.24          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 11       | 1.24          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 4        | 1.24          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 16       | 1.24          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 19       | 1.24          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 4        | 1.24          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 16       | 1.24          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 19       | 1.24          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 17       | 1.24          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 8        | 1.24          |
| (1,785)  | 1:113:A:GLN:HG2 | 1:110:A:PRO:HB2 | 15       | 1.24          |
| (1,652)  | 1:16:A:PHE:H    | 1:64:A:LEU:HD22 | 15       | 1.24          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3  | 5        | 1.24          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 11       | 1.23          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 11       | 1.23          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 1        | 1.23          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 9        | 1.23          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 12       | 1.23          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 11       | 1.23          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 17       | 1.23          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 17       | 1.23          |
| (2,456)  | 1:96:A:GLN:H    | 1:95:A:HIS:H    | 3        | 1.23          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 1        | 1.23          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 7        | 1.23          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 9        | 1.23          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 12       | 1.23          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 1        | 1.23          |
| (1,496)  | 1:96:A:GLN:H    | 1:95:A:HIS:H    | 3        | 1.23          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3  | 10       | 1.23          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3  | 14       | 1.23          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,1124) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB  | 6        | 1.22          |
| (2,1086) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB  | 18       | 1.22          |
| (2,1044) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB  | 6        | 1.22          |
| (2,1019) | 1:38:A:PRO:CB  | 1:96:A:GLN:CB  | 4        | 1.22          |
| (2,1001) | 1:37:A:PRO:CB  | 1:38:A:PRO:CB  | 7        | 1.22          |
| (2,1001) | 1:37:A:PRO:CB  | 1:38:A:PRO:CB  | 8        | 1.22          |
| (2,1001) | 1:37:A:PRO:CB  | 1:38:A:PRO:CB  | 12       | 1.22          |
| (2,975)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB  | 2        | 1.22          |
| (2,975)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB  | 7        | 1.22          |
| (2,975)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB  | 8        | 1.22          |
| (2,958)  | 1:64:A:LEU:H   | 1:65:A:PRO:CB  | 8        | 1.22          |
| (2,854)  | 1:14:A:THR:CA  | 1:66:A:ARG:CB  | 13       | 1.22          |
| (2,752)  | 1:99:A:THR:H   | 1:101:A:THR:CB | 3        | 1.22          |
| (2,746)  | 1:118:A:THR:CB | 1:120:A:PHE:CB | 3        | 1.22          |
| (2,746)  | 1:118:A:THR:CB | 1:120:A:PHE:CB | 3        | 1.22          |
| (2,723)  | 1:86:A:LEU:H   | 1:45:A:TRP:CB  | 4        | 1.22          |
| (2,723)  | 1:86:A:LEU:H   | 1:45:A:TRP:CB  | 19       | 1.22          |
| (2,641)  | 1:47:A:ARG:CB  | 1:67:A:TRP:CB  | 5        | 1.22          |
| (2,565)  | 1:66:A:ARG:H   | 1:67:A:TRP:CB  | 2        | 1.22          |
| (2,563)  | 1:42:A:LYS:H   | 1:71:A:TYR:CB  | 16       | 1.22          |
| (2,415)  | 1:44:A:TYR:H   | 1:92:A:VAL:CB  | 12       | 1.22          |
| (2,403)  | 1:105:A:VAL:H  | 1:74:A:THR:CB  | 2        | 1.22          |
| (2,216)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB  | 2        | 1.22          |
| (2,216)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB  | 7        | 1.22          |
| (2,216)  | 1:42:A:LYS:H   | 1:30:A:VAL:CB  | 8        | 1.22          |
| (2,5)    | 1:44:A:TYR:H   | 1:91:A:TRP:CB  | 12       | 1.22          |
| (1,1294) | 1:63:A:LEU:HG  | 1:61:A:LYS:HG3 | 18       | 1.22          |
| (1,954)  | 1:14:A:THR:HA  | 1:66:A:ARG:HG2 | 19       | 1.22          |
| (2,1139) | 1:9:A:TRP:CB   | 1:108:A:ARG:CB | 16       | 1.21          |
| (2,1124) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB  | 1        | 1.21          |
| (2,1082) | 1:100:A:SER:H  | 1:42:A:LYS:CB  | 12       | 1.21          |
| (2,1065) | 1:9:A:TRP:CB   | 1:108:A:ARG:CB | 16       | 1.21          |
| (2,1044) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB  | 1        | 1.21          |
| (2,1001) | 1:37:A:PRO:CB  | 1:38:A:PRO:CB  | 6        | 1.21          |
| (2,1001) | 1:37:A:PRO:CB  | 1:38:A:PRO:CB  | 9        | 1.21          |
| (2,1001) | 1:37:A:PRO:CB  | 1:38:A:PRO:CB  | 14       | 1.21          |
| (2,1001) | 1:37:A:PRO:CB  | 1:38:A:PRO:CB  | 17       | 1.21          |
| (2,920)  | 1:9:A:TRP:CB   | 1:108:A:ARG:CB | 16       | 1.21          |
| (2,808)  | 1:20:A:ARG:CB  | 1:128:A:GLN:CB | 17       | 1.21          |
| (2,783)  | 1:124:A:THR:CB | 1:24:A:PHE:CB  | 18       | 1.21          |
| (1,1271) | 1:128:A:GLN:HA | 1:20:A:ARG:HG2 | 14       | 1.21          |
| (1,954)  | 1:14:A:THR:HA  | 1:66:A:ARG:HG2 | 3        | 1.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 12       | 1.21          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 10       | 1.21          |
| (1,62)   | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 5        | 1.21          |
| (2,1018) | 1:50:A:ARG:CB   | 1:66:A:ARG:CB   | 5        | 1.2           |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 15       | 1.2           |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 8        | 1.2           |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 8        | 1.2           |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 4        | 1.2           |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 7        | 1.2           |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 8        | 1.2           |
| (2,188)  | 1:125:A:ILE:CB  | 1:23:A:LYS:CB   | 9        | 1.2           |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 6        | 1.2           |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 5        | 1.2           |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 19       | 1.2           |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 11       | 1.2           |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 3        | 1.2           |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 2        | 1.19          |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 5        | 1.19          |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 10       | 1.19          |
| (2,999)  | 1:130:A:TYR:H   | 1:13:A:ILE:CB   | 6        | 1.19          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 6        | 1.19          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 16       | 1.19          |
| (2,938)  | 1:44:A:TYR:CB   | 1:72:A:LEU:CB   | 5        | 1.19          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 19       | 1.19          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 10       | 1.19          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 10       | 1.19          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB  | 17       | 1.19          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 1        | 1.19          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 4        | 1.19          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 19       | 1.19          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 15       | 1.19          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 17       | 1.19          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 9        | 1.19          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 18       | 1.19          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 18       | 1.19          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 6        | 1.19          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 12       | 1.19          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 13       | 1.19          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 4        | 1.19          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 1        | 1.19          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 19       | 1.19          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 8        | 1.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 6        | 1.19          |
| (1,641)  | 1:108:A:ARG:HB3  | 1:9:A:TRP:HE1   | 11       | 1.19          |
| (1,414)  | 1:65:A:PRO:HB3   | 1:67:A:TRP:HE1  | 11       | 1.19          |
| (1,346)  | 1:43:A:GLY:HA3   | 1:72:A:LEU:HA   | 11       | 1.19          |
| (1,346)  | 1:43:A:GLY:HA3   | 1:72:A:LEU:HA   | 12       | 1.19          |
| (2,1001) | 1:37:A:PRO:CB    | 1:38:A:PRO:CB   | 3        | 1.18          |
| (2,958)  | 1:64:A:LEU:H     | 1:65:A:PRO:CB   | 19       | 1.18          |
| (2,762)  | 1:126:A:LEU:H    | 1:127:A:PRO:CB  | 1        | 1.18          |
| (2,614)  | 1:41:A:ALA:H     | 1:36:A:VAL:CB   | 1        | 1.18          |
| (2,614)  | 1:41:A:ALA:H     | 1:36:A:VAL:CB   | 13       | 1.18          |
| (2,565)  | 1:66:A:ARG:H     | 1:67:A:TRP:CB   | 1        | 1.18          |
| (2,415)  | 1:44:A:TYR:H     | 1:92:A:VAL:CB   | 17       | 1.18          |
| (2,415)  | 1:44:A:TYR:H     | 1:92:A:VAL:CB   | 18       | 1.18          |
| (2,188)  | 1:125:A:ILE:CB   | 1:23:A:LYS:CB   | 1        | 1.18          |
| (2,105)  | 1:24:A:PHE:CA    | 1:125:A:ILE:CB  | 1        | 1.18          |
| (2,56)   | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 9        | 1.18          |
| (2,21)   | 1:128:A:GLN:CB   | 1:20:A:ARG:CB   | 1        | 1.18          |
| (2,5)    | 1:44:A:TYR:H     | 1:91:A:TRP:CB   | 11       | 1.18          |
| (1,1269) | 1:20:A:ARG:HG2   | 1:128:A:GLN:HG3 | 2        | 1.18          |
| (1,349)  | 1:63:A:LEU:H     | 1:52:A:SER:HB2  | 13       | 1.18          |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 5        | 1.18          |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 11       | 1.17          |
| (2,1106) | 1:5:A:PRO:CB     | 1:4:A:ILE:CA    | 2        | 1.17          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 17       | 1.17          |
| (2,999)  | 1:130:A:TYR:H    | 1:13:A:ILE:CB   | 9        | 1.17          |
| (2,891)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB   | 8        | 1.17          |
| (2,641)  | 1:47:A:ARG:CB    | 1:67:A:TRP:CB   | 7        | 1.17          |
| (2,604)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 18       | 1.17          |
| (2,565)  | 1:66:A:ARG:H     | 1:67:A:TRP:CB   | 6        | 1.17          |
| (2,417)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 18       | 1.17          |
| (2,5)    | 1:44:A:TYR:H     | 1:91:A:TRP:CB   | 10       | 1.17          |
| (2,5)    | 1:44:A:TYR:H     | 1:91:A:TRP:CB   | 18       | 1.17          |
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 8        | 1.17          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 2        | 1.16          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 8        | 1.16          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 9        | 1.16          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 12       | 1.16          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 13       | 1.16          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 14       | 1.16          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 18       | 1.16          |
| (2,1105) | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 19       | 1.16          |
| (2,1001) | 1:37:A:PRO:CB    | 1:38:A:PRO:CB   | 18       | 1.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB   | 7        | 1.16          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 6        | 1.16          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 9        | 1.16          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 11       | 1.16          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 16       | 1.16          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 17       | 1.16          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 1        | 1.16          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 18       | 1.16          |
| (2,537)  | 1:124:A:THR:H   | 1:28:A:GLN:CB   | 17       | 1.16          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 1        | 1.16          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 3        | 1.16          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 5        | 1.16          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 6        | 1.16          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 5        | 1.16          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 6        | 1.16          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 6        | 1.16          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 5        | 1.16          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 10       | 1.16          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 13       | 1.16          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 19       | 1.16          |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3  | 9        | 1.16          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 6        | 1.15          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 13       | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 1        | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 3        | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 4        | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 5        | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 6        | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 10       | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 11       | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 15       | 1.15          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 16       | 1.15          |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 1        | 1.15          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 17       | 1.15          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 17       | 1.15          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 17       | 1.15          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 3        | 1.15          |
| (2,537)  | 1:124:A:THR:H   | 1:28:A:GLN:CB   | 18       | 1.15          |
| (2,388)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 16       | 1.15          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 8        | 1.15          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 19       | 1.15          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 5        | 1.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 10       | 1.15          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 15       | 1.15          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 14       | 1.15          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 10       | 1.15          |
| (1,652)  | 1:16:A:PHE:H    | 1:64:A:LEU:HD22 | 10       | 1.15          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 3        | 1.15          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 11       | 1.15          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 5        | 1.14          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 10       | 1.14          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 4        | 1.14          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 10       | 1.14          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 17       | 1.14          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 19       | 1.14          |
| (2,1105) | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 7        | 1.14          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 10       | 1.14          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 11       | 1.14          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 10       | 1.14          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 5        | 1.14          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 11       | 1.14          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 3        | 1.14          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 11       | 1.14          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 19       | 1.14          |
| (2,188)  | 1:125:A:ILE:CB  | 1:23:A:LYS:CB   | 16       | 1.14          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 1        | 1.14          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 16       | 1.14          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 1        | 1.14          |
| (1,62)   | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 4        | 1.14          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 3        | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 7        | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 8        | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 9        | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 11       | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 12       | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 14       | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 15       | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 16       | 1.13          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 18       | 1.13          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 14       | 1.13          |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 16       | 1.13          |
| (2,975)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 18       | 1.13          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 17       | 1.13          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 16       | 1.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 6        | 1.13          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 7        | 1.13          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 11       | 1.13          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 14       | 1.13          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 18       | 1.13          |
| (2,216)  | 1:42:A:LYS:H    | 1:30:A:VAL:CB   | 18       | 1.13          |
| (1,1271) | 1:128:A:GLN:HA  | 1:20:A:ARG:HG2  | 16       | 1.13          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 17       | 1.13          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 2        | 1.13          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 6        | 1.13          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 13       | 1.13          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 15       | 1.13          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 9        | 1.12          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 5        | 1.12          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 10       | 1.12          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 12       | 1.12          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 17       | 1.12          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 13       | 1.12          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 14       | 1.12          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 14       | 1.12          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 19       | 1.12          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 4        | 1.12          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 15       | 1.12          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 6        | 1.12          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 4        | 1.12          |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 10       | 1.12          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 2        | 1.12          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 5        | 1.12          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 6        | 1.12          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 16       | 1.12          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 5        | 1.12          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2 | 15       | 1.12          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 1        | 1.12          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 12       | 1.12          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 10       | 1.12          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 14       | 1.12          |
| (2,1106) | 1:5:A:PRO:CB    | 1:4:A:ILE:CA    | 1        | 1.11          |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 4        | 1.11          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 15       | 1.11          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 15       | 1.11          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 2        | 1.11          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 15       | 1.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 7        | 1.11          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 8        | 1.11          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 2        | 1.11          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 2        | 1.11          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 2        | 1.11          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 5        | 1.11          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 19       | 1.11          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 12       | 1.11          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 9        | 1.11          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 13       | 1.11          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 8        | 1.11          |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 19       | 1.11          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 17       | 1.11          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 19       | 1.11          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 2        | 1.11          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 3        | 1.11          |
| (1,888)  | 1:20:A:ARG:HD2  | 1:128:A:GLN:HG3 | 2        | 1.11          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 1        | 1.11          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 19       | 1.11          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 16       | 1.11          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 18       | 1.11          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 18       | 1.1           |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 11       | 1.1           |
| (2,956)  | 1:9:A:TRP:CB    | 1:107:A:SER:CB  | 17       | 1.1           |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 17       | 1.1           |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 1        | 1.1           |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 1        | 1.1           |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 11       | 1.1           |
| (2,641)  | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 3        | 1.1           |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 6        | 1.1           |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 19       | 1.1           |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 4        | 1.1           |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 2        | 1.1           |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 12       | 1.1           |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 9        | 1.1           |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 18       | 1.1           |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 10       | 1.1           |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 6        | 1.1           |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 10       | 1.1           |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 14       | 1.1           |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 10       | 1.1           |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 14       | 1.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 7        | 1.1           |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 17       | 1.1           |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 2        | 1.1           |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 16       | 1.1           |
| (1,1227) | 1:105:A:VAL:HA  | 1:103:A:SER:HB2 | 13       | 1.1           |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 4        | 1.1           |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 5        | 1.1           |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3  | 3        | 1.1           |
| (1,599)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD22 | 14       | 1.1           |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2  | 2        | 1.1           |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 17       | 1.1           |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 6        | 1.09          |
| (2,1001) | 1:37:A:PRO:CB   | 1:38:A:PRO:CB   | 19       | 1.09          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 13       | 1.09          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 2        | 1.09          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 8        | 1.09          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 9        | 1.09          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 12       | 1.09          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 13       | 1.09          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 18       | 1.09          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 19       | 1.09          |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB   | 3        | 1.09          |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB   | 17       | 1.09          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 10       | 1.09          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 6        | 1.09          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 9        | 1.09          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 9        | 1.09          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 13       | 1.09          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 19       | 1.09          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 8        | 1.09          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 9        | 1.09          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 9        | 1.09          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 18       | 1.09          |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB   | 17       | 1.09          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 6        | 1.09          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 6        | 1.09          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 13       | 1.09          |
| (2,152)  | 1:7:A:TYR:CB    | 1:110:A:PRO:CB  | 17       | 1.09          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 7        | 1.09          |
| (2,85)   | 1:45:A:TRP:CB   | 1:91:A:TRP:CB   | 2        | 1.09          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 1        | 1.09          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 4        | 1.09          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1363) | 1:52:A:SER:HB2   | 1:62:A:GLN:HG2  | 9        | 1.09          |
| (1,1269) | 1:20:A:ARG:HG2   | 1:128:A:GLN:HG3 | 8        | 1.09          |
| (1,1269) | 1:20:A:ARG:HG2   | 1:128:A:GLN:HG3 | 13       | 1.09          |
| (1,1163) | 1:113:A:GLN:HG3  | 1:110:A:PRO:HB2 | 10       | 1.09          |
| (1,888)  | 1:20:A:ARG:HD2   | 1:128:A:GLN:HG3 | 11       | 1.09          |
| (1,888)  | 1:20:A:ARG:HD2   | 1:128:A:GLN:HG3 | 12       | 1.09          |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 8        | 1.09          |
| (2,1163) | 1:99:A:THR:H     | 1:42:A:LYS:CB   | 15       | 1.08          |
| (2,1163) | 1:99:A:THR:H     | 1:42:A:LYS:CB   | 17       | 1.08          |
| (2,999)  | 1:130:A:TYR:H    | 1:13:A:ILE:CB   | 8        | 1.08          |
| (2,961)  | 1:120:A:PHE:H    | 1:121:A:PRO:CB  | 11       | 1.08          |
| (2,956)  | 1:9:A:TRP:CB     | 1:107:A:SER:CB  | 2        | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 1        | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 3        | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 4        | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 6        | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 10       | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 11       | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 14       | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 15       | 1.08          |
| (2,955)  | 1:116:A:ILE:CA   | 1:117:A:PRO:CB  | 16       | 1.08          |
| (2,746)  | 1:118:A:THR:CB   | 1:120:A:PHE:CB  | 4        | 1.08          |
| (2,746)  | 1:118:A:THR:CB   | 1:120:A:PHE:CB  | 4        | 1.08          |
| (2,689)  | 1:106:A:SER:H    | 1:9:A:TRP:CB    | 16       | 1.08          |
| (2,596)  | 1:93:A:ALA:CB    | 1:99:A:THR:CB   | 14       | 1.08          |
| (2,596)  | 1:93:A:ALA:CB    | 1:99:A:THR:CB   | 15       | 1.08          |
| (2,596)  | 1:93:A:ALA:CB    | 1:99:A:THR:CB   | 18       | 1.08          |
| (2,518)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 2        | 1.08          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 4        | 1.08          |
| (2,442)  | 1:37:A:PRO:CB    | 1:36:A:VAL:CB   | 16       | 1.08          |
| (2,415)  | 1:44:A:TYR:H     | 1:92:A:VAL:CB   | 6        | 1.08          |
| (2,333)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 3        | 1.08          |
| (2,333)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 9        | 1.08          |
| (2,333)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 13       | 1.08          |
| (2,333)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 17       | 1.08          |
| (2,316)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 3        | 1.08          |
| (2,316)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 9        | 1.08          |
| (2,316)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 13       | 1.08          |
| (2,316)  | 1:36:A:VAL:H     | 1:37:A:PRO:CB   | 17       | 1.08          |
| (2,285)  | 1:46:A:TYR:CB    | 1:68:A:TYR:CB   | 4        | 1.08          |
| (2,105)  | 1:24:A:PHE:CA    | 1:125:A:ILE:CB  | 15       | 1.08          |
| (2,56)   | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 15       | 1.08          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 1        | 1.08          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 13       | 1.08          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 18       | 1.08          |
| (1,1269) | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 12       | 1.08          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 10       | 1.08          |
| (1,1227) | 1:105:A:VAL:HA  | 1:103:A:SER:HB2 | 11       | 1.08          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 7        | 1.08          |
| (1,770)  | 1:111:A:THR:HB  | 1:110:A:PRO:HG3 | 11       | 1.08          |
| (1,133)  | 1:26:A:ASP:HA   | 1:27:A:GLY:H    | 18       | 1.08          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 4        | 1.08          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 4        | 1.07          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 7        | 1.07          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 3        | 1.07          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 14       | 1.07          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 1        | 1.07          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 5        | 1.07          |
| (2,955)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 7        | 1.07          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 11       | 1.07          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 14       | 1.07          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 19       | 1.07          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB  | 2        | 1.07          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 11       | 1.07          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 9        | 1.07          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 11       | 1.07          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 18       | 1.07          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 8        | 1.07          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 17       | 1.07          |
| (2,442)  | 1:37:A:PRO:CB   | 1:36:A:VAL:CB   | 19       | 1.07          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 2        | 1.07          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 2        | 1.07          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 14       | 1.07          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 1        | 1.07          |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 6        | 1.07          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 8        | 1.07          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 6        | 1.07          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 15       | 1.07          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 15       | 1.07          |
| (1,788)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE22 | 15       | 1.07          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 5        | 1.07          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 12       | 1.07          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 3        | 1.06          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 18       | 1.06          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 18       | 1.06          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 1        | 1.06          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 15       | 1.06          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 7        | 1.06          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 9        | 1.06          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 18       | 1.06          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 8        | 1.06          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 3        | 1.06          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 8        | 1.06          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 15       | 1.06          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 4        | 1.06          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 5        | 1.06          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 5        | 1.06          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 18       | 1.06          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 18       | 1.06          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 3        | 1.06          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 2        | 1.06          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 5        | 1.06          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 14       | 1.06          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 7        | 1.06          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 10       | 1.06          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 12       | 1.06          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 18       | 1.06          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 14       | 1.06          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 14       | 1.06          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 10       | 1.06          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 19       | 1.06          |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 14       | 1.06          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 18       | 1.06          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 13       | 1.06          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 3        | 1.06          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 6        | 1.06          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 7        | 1.06          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 16       | 1.06          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 18       | 1.06          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 11       | 1.06          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 14       | 1.06          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 14       | 1.06          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 14       | 1.06          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 16       | 1.06          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 16       | 1.06          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 14       | 1.06          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 14       | 1.06          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 8        | 1.05          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 2        | 1.05          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 3        | 1.05          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 12       | 1.05          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 12       | 1.05          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 3        | 1.05          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 9        | 1.05          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 9        | 1.05          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB    | 13       | 1.05          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 10       | 1.05          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 12       | 1.05          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 17       | 1.05          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 18       | 1.05          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 8        | 1.05          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 16       | 1.05          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 1        | 1.05          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 1        | 1.05          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 12       | 1.05          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 7        | 1.05          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 4        | 1.05          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 6        | 1.05          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 13       | 1.05          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 17       | 1.05          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 19       | 1.05          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 9        | 1.05          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 12       | 1.05          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 13       | 1.05          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 17       | 1.05          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 4        | 1.05          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 4        | 1.05          |
| (1,599)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD22 | 5        | 1.05          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 19       | 1.05          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 14       | 1.04          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 10       | 1.04          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 16       | 1.04          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 17       | 1.04          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 19       | 1.04          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB   | 2        | 1.04          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 7        | 1.04          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 7        | 1.04          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 1        | 1.04          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 17       | 1.04          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 6        | 1.04          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 7        | 1.04          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 13       | 1.04          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 1        | 1.04          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 17       | 1.04          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 4        | 1.04          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 7        | 1.04          |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB   | 2        | 1.04          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 11       | 1.04          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 11       | 1.04          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 1        | 1.04          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 10       | 1.04          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 15       | 1.04          |
| (1,599)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD22 | 12       | 1.04          |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2  | 11       | 1.04          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 18       | 1.04          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 2        | 1.03          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 2        | 1.03          |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 3        | 1.03          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 4        | 1.03          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 9        | 1.03          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 1        | 1.03          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 13       | 1.03          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 13       | 1.03          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 16       | 1.03          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 8        | 1.03          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 19       | 1.03          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 1        | 1.03          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 12       | 1.03          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 2        | 1.03          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 11       | 1.03          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 6        | 1.03          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 9        | 1.03          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 4        | 1.03          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 16       | 1.03          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 8        | 1.03          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 19       | 1.03          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 4        | 1.03          |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB   | 18       | 1.03          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 11       | 1.03          |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 15       | 1.03          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 14       | 1.03          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 5        | 1.03          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 16       | 1.03          |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 1        | 1.03          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 11       | 1.03          |
| (2,2)    | 1:45:A:TRP:CB   | 1:44:A:TYR:CB   | 19       | 1.03          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 9        | 1.03          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 8        | 1.03          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 8        | 1.03          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 13       | 1.03          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 15       | 1.03          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 9        | 1.03          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 16       | 1.03          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 5        | 1.02          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 12       | 1.02          |
| (2,1018) | 1:50:A:ARG:CB   | 1:66:A:ARG:CB   | 17       | 1.02          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 12       | 1.02          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 7        | 1.02          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 7        | 1.02          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 4        | 1.02          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 11       | 1.02          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 11       | 1.02          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 15       | 1.02          |
| (2,746)  | 1:118:A:THR:CB  | 1:120:A:PHE:CB  | 15       | 1.02          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB  | 13       | 1.02          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 16       | 1.02          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 17       | 1.02          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 19       | 1.02          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 11       | 1.02          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 15       | 1.02          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 8        | 1.02          |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 13       | 1.02          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 10       | 1.02          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 13       | 1.02          |
| (2,518)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 6        | 1.02          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 11       | 1.02          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 15       | 1.02          |
| (2,406)  | 1:33:A:ALA:CB   | 1:71:A:TYR:CB   | 12       | 1.02          |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB   | 15       | 1.02          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 14       | 1.02          |
| (2,106)  | 1:68:A:TYR:CB   | 1:66:A:ARG:CB   | 13       | 1.02          |
| (2,86)   | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 5        | 1.02          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 7        | 1.02          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 8        | 1.02          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 11       | 1.02          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 12       | 1.02          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 15       | 1.02          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 16       | 1.02          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 18       | 1.02          |
| (2,76)   | 1:46:A:TYR:CB    | 1:76:A:PRO:CB   | 10       | 1.02          |
| (2,2)    | 1:45:A:TRP:CB    | 1:44:A:TYR:CB   | 8        | 1.02          |
| (2,2)    | 1:45:A:TRP:CB    | 1:44:A:TYR:CB   | 14       | 1.02          |
| (1,954)  | 1:14:A:THR:HA    | 1:66:A:ARG:HG2  | 11       | 1.02          |
| (1,720)  | 1:70:A:TYR:H     | 1:31:A:PRO:HG2  | 11       | 1.02          |
| (1,599)  | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD22 | 7        | 1.02          |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 15       | 1.02          |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 6        | 1.01          |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 14       | 1.01          |
| (2,961)  | 1:120:A:PHE:H    | 1:121:A:PRO:CB  | 5        | 1.01          |
| (2,958)  | 1:64:A:LEU:H     | 1:65:A:PRO:CB   | 6        | 1.01          |
| (2,839)  | 1:69:A:PHE:CB    | 1:31:A:PRO:CB   | 5        | 1.01          |
| (2,825)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB   | 7        | 1.01          |
| (2,746)  | 1:118:A:THR:CB   | 1:120:A:PHE:CB  | 16       | 1.01          |
| (2,746)  | 1:118:A:THR:CB   | 1:120:A:PHE:CB  | 16       | 1.01          |
| (2,727)  | 1:114:A:GLU:CB   | 1:116:A:ILE:CB  | 9        | 1.01          |
| (2,723)  | 1:86:A:LEU:H     | 1:45:A:TRP:CB   | 13       | 1.01          |
| (2,689)  | 1:106:A:SER:H    | 1:9:A:TRP:CB    | 1        | 1.01          |
| (2,604)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 4        | 1.01          |
| (2,604)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 7        | 1.01          |
| (2,604)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 14       | 1.01          |
| (2,594)  | 1:29:A:GLY:H     | 1:92:A:VAL:CB   | 11       | 1.01          |
| (2,417)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 4        | 1.01          |
| (2,417)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 7        | 1.01          |
| (2,417)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 14       | 1.01          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 3        | 1.01          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 7        | 1.01          |
| (2,285)  | 1:46:A:TYR:CB    | 1:68:A:TYR:CB   | 2        | 1.01          |
| (2,239)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 15       | 1.01          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 3        | 1.01          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 9        | 1.01          |
| (2,84)   | 1:44:A:TYR:CB    | 1:91:A:TRP:CB   | 11       | 1.01          |
| (2,84)   | 1:44:A:TYR:CB    | 1:91:A:TRP:CB   | 12       | 1.01          |
| (2,84)   | 1:44:A:TYR:CB    | 1:91:A:TRP:CB   | 15       | 1.01          |
| (2,84)   | 1:44:A:TYR:CB    | 1:91:A:TRP:CB   | 19       | 1.01          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,56)   | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 17       | 1.01          |
| (2,2)    | 1:45:A:TRP:CB    | 1:44:A:TYR:CB   | 17       | 1.01          |
| (1,1278) | 1:78:A:ALA:HA    | 1:76:A:PRO:HD3  | 14       | 1.01          |
| (1,1154) | 1:11:A:SER:HA    | 1:136:A:GLY:HA3 | 13       | 1.01          |
| (1,851)  | 1:28:A:GLN:H     | 1:25:A:SER:HB3  | 7        | 1.01          |
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 13       | 1.01          |
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 17       | 1.01          |
| (1,53)   | 1:138:A:SER:HA   | 1:11:A:SER:HB3  | 15       | 1.01          |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 6        | 1.01          |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 14       | 1.01          |
| (2,854)  | 1:14:A:THR:CA    | 1:66:A:ARG:CB   | 9        | 1.0           |
| (2,641)  | 1:47:A:ARG:CB    | 1:67:A:TRP:CB   | 8        | 1.0           |
| (2,604)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 2        | 1.0           |
| (2,604)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 3        | 1.0           |
| (2,604)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 13       | 1.0           |
| (2,417)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 2        | 1.0           |
| (2,417)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 3        | 1.0           |
| (2,417)  | 1:30:A:VAL:H     | 1:31:A:PRO:CB   | 13       | 1.0           |
| (2,285)  | 1:46:A:TYR:CB    | 1:68:A:TYR:CB   | 9        | 1.0           |
| (2,239)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 19       | 1.0           |
| (2,188)  | 1:125:A:ILE:CB   | 1:23:A:LYS:CB   | 4        | 1.0           |
| (2,102)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB   | 8        | 1.0           |
| (2,2)    | 1:45:A:TRP:CB    | 1:44:A:TYR:CB   | 9        | 1.0           |
| (1,1294) | 1:63:A:LEU:HG    | 1:61:A:LYS:HG3  | 4        | 1.0           |
| (1,1269) | 1:20:A:ARG:HG2   | 1:128:A:GLN:HG3 | 14       | 1.0           |
| (1,954)  | 1:14:A:THR:HA    | 1:66:A:ARG:HG2  | 16       | 1.0           |
| (1,770)  | 1:111:A:THR:HB   | 1:110:A:PRO:HG3 | 18       | 1.0           |
| (1,736)  | 1:113:A:GLN:HA   | 1:108:A:ARG:HD2 | 16       | 1.0           |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 9        | 0.99          |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 13       | 0.99          |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 19       | 0.99          |
| (2,1163) | 1:99:A:THR:H     | 1:42:A:LYS:CB   | 8        | 0.99          |
| (2,891)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB   | 11       | 0.99          |
| (2,886)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB   | 5        | 0.99          |
| (2,860)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB   | 5        | 0.99          |
| (2,839)  | 1:69:A:PHE:CB    | 1:31:A:PRO:CB   | 12       | 0.99          |
| (2,792)  | 1:108:A:ARG:H    | 1:9:A:TRP:CB    | 19       | 0.99          |
| (2,783)  | 1:124:A:THR:CB   | 1:24:A:PHE:CB   | 5        | 0.99          |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 15       | 0.99          |
| (2,746)  | 1:118:A:THR:CB   | 1:120:A:PHE:CB  | 19       | 0.99          |
| (2,746)  | 1:118:A:THR:CB   | 1:120:A:PHE:CB  | 19       | 0.99          |
| (2,651)  | 1:70:A:TYR:H     | 1:31:A:PRO:CB   | 4        | 0.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 8        | 0.99          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 16       | 0.99          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 2        | 0.99          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 16       | 0.99          |
| (2,415)  | 1:44:A:TYR:H    | 1:92:A:VAL:CB   | 16       | 0.99          |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB   | 11       | 0.99          |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB   | 19       | 0.99          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 5        | 0.99          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 18       | 0.99          |
| (2,152)  | 1:7:A:TYR:CB    | 1:110:A:PRO:CB  | 8        | 0.99          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 19       | 0.99          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 9        | 0.99          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 13       | 0.99          |
| (1,413)  | 1:94:A:ASN:HD22 | 1:96:A:GLN:HB3  | 19       | 0.99          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 15       | 0.99          |
| (1,334)  | 1:138:A:SER:H   | 1:134:A:GLY:HA3 | 16       | 0.99          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 7        | 0.99          |
| (1,97)   | 1:32:A:ILE:HG23 | 1:119:A:ARG:HB3 | 8        | 0.99          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 7        | 0.98          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 12       | 0.98          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 17       | 0.98          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 16       | 0.98          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 6        | 0.98          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 10       | 0.98          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB    | 9        | 0.98          |
| (2,776)  | 1:28:A:GLN:H    | 1:30:A:VAL:CB   | 2        | 0.98          |
| (2,776)  | 1:28:A:GLN:H    | 1:30:A:VAL:CB   | 19       | 0.98          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 4        | 0.98          |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 10       | 0.98          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 1        | 0.98          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 15       | 0.98          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB   | 18       | 0.98          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 5        | 0.98          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 19       | 0.98          |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 10       | 0.98          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 15       | 0.98          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 15       | 0.98          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 3        | 0.98          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 8        | 0.98          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 9        | 0.98          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 8        | 0.98          |
| (1,785)  | 1:113:A:GLN:HG2 | 1:110:A:PRO:HB2 | 7        | 0.98          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,710)  | 1:47:A:ARG:HG2   | 1:67:A:TRP:HE1  | 4        | 0.98          |
| (1,349)  | 1:63:A:LEU:H     | 1:52:A:SER:HB2  | 17       | 0.98          |
| (1,53)   | 1:138:A:SER:HA   | 1:11:A:SER:HB3  | 6        | 0.98          |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 18       | 0.97          |
| (2,1163) | 1:99:A:THR:H     | 1:42:A:LYS:CB   | 3        | 0.97          |
| (2,1139) | 1:9:A:TRP:CB     | 1:108:A:ARG:CB  | 19       | 0.97          |
| (2,1086) | 1:47:A:ARG:CB    | 1:67:A:TRP:CB   | 2        | 0.97          |
| (2,1065) | 1:9:A:TRP:CB     | 1:108:A:ARG:CB  | 19       | 0.97          |
| (2,920)  | 1:9:A:TRP:CB     | 1:108:A:ARG:CB  | 19       | 0.97          |
| (2,854)  | 1:14:A:THR:CA    | 1:66:A:ARG:CB   | 6        | 0.97          |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 1        | 0.97          |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 4        | 0.97          |
| (2,752)  | 1:99:A:THR:H     | 1:101:A:THR:CB  | 14       | 0.97          |
| (2,727)  | 1:114:A:GLU:CB   | 1:116:A:ILE:CB  | 19       | 0.97          |
| (2,723)  | 1:86:A:LEU:H     | 1:45:A:TRP:CB   | 8        | 0.97          |
| (2,651)  | 1:70:A:TYR:H     | 1:31:A:PRO:CB   | 8        | 0.97          |
| (2,614)  | 1:41:A:ALA:H     | 1:36:A:VAL:CB   | 18       | 0.97          |
| (2,587)  | 1:81:A:SER:CB    | 1:84:A:GLU:CB   | 7        | 0.97          |
| (2,563)  | 1:42:A:LYS:H     | 1:71:A:TYR:CB   | 14       | 0.97          |
| (2,415)  | 1:44:A:TYR:H     | 1:92:A:VAL:CB   | 5        | 0.97          |
| (2,379)  | 1:121:A:PRO:CA   | 1:32:A:ILE:CB   | 17       | 0.97          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 4        | 0.97          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 8        | 0.97          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 16       | 0.97          |
| (2,285)  | 1:46:A:TYR:CB    | 1:68:A:TYR:CB   | 16       | 0.97          |
| (2,198)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 3        | 0.97          |
| (2,198)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 9        | 0.97          |
| (2,198)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 10       | 0.97          |
| (2,198)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 11       | 0.97          |
| (2,198)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 13       | 0.97          |
| (2,198)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 15       | 0.97          |
| (2,198)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 16       | 0.97          |
| (2,84)   | 1:44:A:TYR:CB    | 1:91:A:TRP:CB   | 10       | 0.97          |
| (1,954)  | 1:14:A:THR:HA    | 1:66:A:ARG:HG2  | 6        | 0.97          |
| (1,780)  | 1:131:A:TYR:H    | 1:16:A:PHE:HB3  | 15       | 0.97          |
| (1,349)  | 1:63:A:LEU:H     | 1:52:A:SER:HB2  | 5        | 0.97          |
| (1,346)  | 1:43:A:GLY:HA3   | 1:72:A:LEU:HA   | 2        | 0.97          |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 16       | 0.97          |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 16       | 0.97          |
| (2,1202) | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 16       | 0.96          |
| (2,1086) | 1:47:A:ARG:CB    | 1:67:A:TRP:CB   | 4        | 0.96          |
| (2,1086) | 1:47:A:ARG:CB    | 1:67:A:TRP:CB   | 17       | 0.96          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,891)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 17       | 0.96          |
| (2,776)  | 1:28:A:GLN:H   | 1:30:A:VAL:CB   | 14       | 0.96          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB  | 12       | 0.96          |
| (2,370)  | 1:75:A:GLY:H   | 1:76:A:PRO:CB   | 6        | 0.96          |
| (2,239)  | 1:94:A:ASN:CB  | 1:96:A:GLN:CB   | 2        | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 1        | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 4        | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 5        | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 7        | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 8        | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 12       | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 14       | 0.96          |
| (2,198)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB  | 19       | 0.96          |
| (2,2)    | 1:45:A:TRP:CB  | 1:44:A:TYR:CB   | 5        | 0.96          |
| (1,1334) | 1:16:A:PHE:HB3 | 1:130:A:TYR:HB3 | 10       | 0.96          |
| (1,1271) | 1:128:A:GLN:HA | 1:20:A:ARG:HG2  | 10       | 0.96          |
| (1,1154) | 1:11:A:SER:HA  | 1:136:A:GLY:HA3 | 2        | 0.96          |
| (1,1005) | 1:135:A:SER:HA | 1:117:A:PRO:HD2 | 19       | 0.96          |
| (1,736)  | 1:113:A:GLN:HA | 1:108:A:ARG:HD2 | 5        | 0.96          |
| (1,690)  | 1:99:A:THR:HA  | 1:42:A:LYS:HB3  | 1        | 0.96          |
| (1,86)   | 1:101:A:THR:HB | 1:100:A:SER:HB3 | 4        | 0.96          |
| (2,1139) | 1:9:A:TRP:CB   | 1:108:A:ARG:CB  | 6        | 0.95          |
| (2,1123) | 1:126:A:LEU:CB | 1:13:A:ILE:CB   | 10       | 0.95          |
| (2,1123) | 1:126:A:LEU:CB | 1:13:A:ILE:CB   | 12       | 0.95          |
| (2,1065) | 1:9:A:TRP:CB   | 1:108:A:ARG:CB  | 6        | 0.95          |
| (2,920)  | 1:9:A:TRP:CB   | 1:108:A:ARG:CB  | 6        | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 3        | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 6        | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 7        | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 8        | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 10       | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 12       | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 13       | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 14       | 0.95          |
| (2,901)  | 1:37:A:PRO:CA  | 1:38:A:PRO:CB   | 17       | 0.95          |
| (2,854)  | 1:14:A:THR:CA  | 1:66:A:ARG:CB   | 5        | 0.95          |
| (2,776)  | 1:28:A:GLN:H   | 1:30:A:VAL:CB   | 7        | 0.95          |
| (2,766)  | 1:120:A:PHE:CA | 1:121:A:PRO:CB  | 1        | 0.95          |
| (2,766)  | 1:120:A:PHE:CA | 1:121:A:PRO:CB  | 2        | 0.95          |
| (2,766)  | 1:120:A:PHE:CA | 1:121:A:PRO:CB  | 3        | 0.95          |
| (2,766)  | 1:120:A:PHE:CA | 1:121:A:PRO:CB  | 4        | 0.95          |
| (2,766)  | 1:120:A:PHE:CA | 1:121:A:PRO:CB  | 5        | 0.95          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 10       | 0.95          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 12       | 0.95          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 13       | 0.95          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 14       | 0.95          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 15       | 0.95          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 16       | 0.95          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 17       | 0.95          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 19       | 0.95          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB  | 18       | 0.95          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 14       | 0.95          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 14       | 0.95          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 15       | 0.95          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 15       | 0.95          |
| (2,596)  | 1:93:A:ALA:CB   | 1:99:A:THR:CB   | 3        | 0.95          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 7        | 0.95          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 3        | 0.95          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 10       | 0.95          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB   | 13       | 0.95          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 15       | 0.95          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 8        | 0.95          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB   | 2        | 0.95          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 8        | 0.95          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 1        | 0.95          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 7        | 0.95          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 12       | 0.95          |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 17       | 0.95          |
| (2,198)  | 1:126:A:LEU:CA  | 1:127:A:PRO:CB  | 2        | 0.95          |
| (2,198)  | 1:126:A:LEU:CA  | 1:127:A:PRO:CB  | 6        | 0.95          |
| (2,198)  | 1:126:A:LEU:CA  | 1:127:A:PRO:CB  | 18       | 0.95          |
| (2,76)   | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 4        | 0.95          |
| (1,1199) | 1:9:A:TRP:HE1   | 1:108:A:ARG:HD3 | 13       | 0.95          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 12       | 0.95          |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 1        | 0.95          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 8        | 0.95          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 14       | 0.95          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 1        | 0.94          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB  | 13       | 0.94          |
| (2,956)  | 1:9:A:TRP:CB    | 1:107:A:SER:CB  | 10       | 0.94          |
| (2,901)  | 1:37:A:PRO:CA   | 1:38:A:PRO:CB   | 1        | 0.94          |
| (2,901)  | 1:37:A:PRO:CA   | 1:38:A:PRO:CB   | 2        | 0.94          |
| (2,901)  | 1:37:A:PRO:CA   | 1:38:A:PRO:CB   | 4        | 0.94          |
| (2,901)  | 1:37:A:PRO:CA   | 1:38:A:PRO:CB   | 5        | 0.94          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,901) | 1:37:A:PRO:CA  | 1:38:A:PRO:CB  | 9        | 0.94          |
| (2,901) | 1:37:A:PRO:CA  | 1:38:A:PRO:CB  | 15       | 0.94          |
| (2,901) | 1:37:A:PRO:CA  | 1:38:A:PRO:CB  | 18       | 0.94          |
| (2,891) | 1:48:A:HIS:CB  | 1:68:A:TYR:CB  | 18       | 0.94          |
| (2,854) | 1:14:A:THR:CA  | 1:66:A:ARG:CB  | 8        | 0.94          |
| (2,841) | 1:71:A:TYR:CB  | 1:105:A:VAL:CB | 5        | 0.94          |
| (2,776) | 1:28:A:GLN:H   | 1:30:A:VAL:CB  | 5        | 0.94          |
| (2,766) | 1:120:A:PHE:CA | 1:121:A:PRO:CB | 11       | 0.94          |
| (2,762) | 1:126:A:LEU:H  | 1:127:A:PRO:CB | 9        | 0.94          |
| (2,727) | 1:114:A:GLU:CB | 1:116:A:ILE:CB | 11       | 0.94          |
| (2,641) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB  | 9        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 2        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 2        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 4        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 4        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 5        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 5        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 6        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 6        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 7        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 7        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 9        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 9        | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 16       | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 16       | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 17       | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 17       | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 18       | 0.94          |
| (2,629) | 1:101:A:THR:CA | 1:102:A:PRO:CB | 18       | 0.94          |
| (2,604) | 1:30:A:VAL:H   | 1:31:A:PRO:CB  | 5        | 0.94          |
| (2,593) | 1:16:A:PHE:H   | 1:64:A:LEU:CB  | 17       | 0.94          |
| (2,417) | 1:30:A:VAL:H   | 1:31:A:PRO:CB  | 5        | 0.94          |
| (2,406) | 1:33:A:ALA:CB  | 1:71:A:TYR:CB  | 19       | 0.94          |
| (2,379) | 1:121:A:PRO:CA | 1:32:A:ILE:CB  | 10       | 0.94          |
| (2,370) | 1:75:A:GLY:H   | 1:76:A:PRO:CB  | 9        | 0.94          |
| (2,370) | 1:75:A:GLY:H   | 1:76:A:PRO:CB  | 14       | 0.94          |
| (2,324) | 1:63:A:LEU:H   | 1:52:A:SER:CB  | 5        | 0.94          |
| (2,285) | 1:46:A:TYR:CB  | 1:68:A:TYR:CB  | 6        | 0.94          |
| (2,285) | 1:46:A:TYR:CB  | 1:68:A:TYR:CB  | 17       | 0.94          |
| (2,239) | 1:94:A:ASN:CB  | 1:96:A:GLN:CB  | 7        | 0.94          |
| (2,239) | 1:94:A:ASN:CB  | 1:96:A:GLN:CB  | 10       | 0.94          |
| (2,198) | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 17       | 0.94          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 18       | 0.94          |
| (2,6)    | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 19       | 0.94          |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 15       | 0.94          |
| (1,1269) | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 9        | 0.94          |
| (1,1227) | 1:105:A:VAL:HA  | 1:103:A:SER:HB2 | 1        | 0.94          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 2        | 0.94          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 10       | 0.94          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 3        | 0.94          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 3        | 0.94          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 10       | 0.94          |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 10       | 0.94          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 2        | 0.94          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 8        | 0.94          |
| (2,1163) | 1:99:A:THR:H    | 1:42:A:LYS:CB   | 10       | 0.93          |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 13       | 0.93          |
| (2,901)  | 1:37:A:PRO:CA   | 1:38:A:PRO:CB   | 16       | 0.93          |
| (2,901)  | 1:37:A:PRO:CA   | 1:38:A:PRO:CB   | 19       | 0.93          |
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 15       | 0.93          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 12       | 0.93          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 13       | 0.93          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 12       | 0.93          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 13       | 0.93          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 12       | 0.93          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 13       | 0.93          |
| (2,776)  | 1:28:A:GLN:H    | 1:30:A:VAL:CB   | 11       | 0.93          |
| (2,776)  | 1:28:A:GLN:H    | 1:30:A:VAL:CB   | 16       | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 3        | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 3        | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 8        | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 8        | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 10       | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 10       | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 13       | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 13       | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 19       | 0.93          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 19       | 0.93          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 9        | 0.93          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 14       | 0.93          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 4        | 0.93          |
| (2,444)  | 1:104:A:ASP:CB  | 1:36:A:VAL:CB   | 14       | 0.93          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB   | 2        | 0.93          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB   | 15       | 0.93          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,406)  | 1:33:A:ALA:CB    | 1:71:A:TYR:CB   | 4        | 0.93          |
| (2,403)  | 1:105:A:VAL:H    | 1:74:A:THR:CB   | 17       | 0.93          |
| (2,379)  | 1:121:A:PRO:CA   | 1:32:A:ILE:CB   | 16       | 0.93          |
| (2,239)  | 1:94:A:ASN:CB    | 1:96:A:GLN:CB   | 13       | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 3        | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 9        | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 10       | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 11       | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 13       | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 14       | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 15       | 0.93          |
| (2,208)  | 1:126:A:LEU:CA   | 1:127:A:PRO:CB  | 16       | 0.93          |
| (2,188)  | 1:125:A:ILE:CB   | 1:23:A:LYS:CB   | 7        | 0.93          |
| (2,188)  | 1:125:A:ILE:CB   | 1:23:A:LYS:CB   | 15       | 0.93          |
| (2,164)  | 1:69:A:PHE:CB    | 1:10:A:PHE:CB   | 12       | 0.93          |
| (2,5)    | 1:44:A:TYR:H     | 1:91:A:TRP:CB   | 3        | 0.93          |
| (1,1333) | 1:130:A:TYR:HB2  | 1:16:A:PHE:HB3  | 4        | 0.93          |
| (1,1269) | 1:20:A:ARG:HG2   | 1:128:A:GLN:HG3 | 18       | 0.93          |
| (1,1154) | 1:11:A:SER:HA    | 1:136:A:GLY:HA3 | 3        | 0.93          |
| (1,844)  | 1:20:A:ARG:HB3   | 1:17:A:GLN:HE21 | 15       | 0.93          |
| (1,780)  | 1:131:A:TYR:H    | 1:16:A:PHE:HB3  | 10       | 0.93          |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 4        | 0.93          |
| (1,86)   | 1:101:A:THR:HB   | 1:100:A:SER:HB3 | 5        | 0.93          |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2  | 13       | 0.93          |
| (2,1163) | 1:99:A:THR:H     | 1:42:A:LYS:CB   | 4        | 0.92          |
| (2,1123) | 1:126:A:LEU:CB   | 1:13:A:ILE:CB   | 2        | 0.92          |
| (2,1123) | 1:126:A:LEU:CB   | 1:13:A:ILE:CB   | 4        | 0.92          |
| (2,1102) | 1:130:A:TYR:H    | 1:17:A:GLN:CB   | 10       | 0.92          |
| (2,901)  | 1:37:A:PRO:CA    | 1:38:A:PRO:CB   | 11       | 0.92          |
| (2,900)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 14       | 0.92          |
| (2,900)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 15       | 0.92          |
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 17       | 0.92          |
| (2,752)  | 1:99:A:THR:H     | 1:101:A:THR:CB  | 18       | 0.92          |
| (2,727)  | 1:114:A:GLU:CB   | 1:116:A:ILE:CB  | 12       | 0.92          |
| (2,629)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 11       | 0.92          |
| (2,629)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 11       | 0.92          |
| (2,614)  | 1:41:A:ALA:H     | 1:36:A:VAL:CB   | 15       | 0.92          |
| (2,594)  | 1:29:A:GLY:H     | 1:92:A:VAL:CB   | 5        | 0.92          |
| (2,565)  | 1:66:A:ARG:H     | 1:67:A:TRP:CB   | 12       | 0.92          |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 5        | 0.92          |
| (2,406)  | 1:33:A:ALA:CB    | 1:71:A:TYR:CB   | 16       | 0.92          |
| (2,285)  | 1:46:A:TYR:CB    | 1:68:A:TYR:CB   | 15       | 0.92          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,263)  | 1:16:A:PHE:CA  | 1:64:A:LEU:CB  | 5        | 0.92          |
| (2,239)  | 1:94:A:ASN:CB  | 1:96:A:GLN:CB  | 4        | 0.92          |
| (2,239)  | 1:94:A:ASN:CB  | 1:96:A:GLN:CB  | 16       | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 1        | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 2        | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 4        | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 5        | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 7        | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 8        | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 12       | 0.92          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 19       | 0.92          |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB | 8        | 0.92          |
| (2,5)    | 1:44:A:TYR:H   | 1:91:A:TRP:CB  | 7        | 0.92          |
| (1,776)  | 1:125:A:ILE:H  | 1:25:A:SER:HB3 | 15       | 0.92          |
| (1,349)  | 1:63:A:LEU:H   | 1:52:A:SER:HB2 | 19       | 0.92          |
| (2,1153) | 1:93:A:ALA:H   | 1:30:A:VAL:CB  | 5        | 0.91          |
| (2,1153) | 1:93:A:ALA:H   | 1:30:A:VAL:CB  | 7        | 0.91          |
| (2,1153) | 1:93:A:ALA:H   | 1:30:A:VAL:CB  | 14       | 0.91          |
| (2,1147) | 1:101:A:THR:CB | 1:102:A:PRO:CB | 8        | 0.91          |
| (2,1147) | 1:101:A:THR:CB | 1:102:A:PRO:CB | 19       | 0.91          |
| (2,1123) | 1:126:A:LEU:CB | 1:13:A:ILE:CB  | 11       | 0.91          |
| (2,1123) | 1:126:A:LEU:CB | 1:13:A:ILE:CB  | 15       | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 2        | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 5        | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 6        | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 7        | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 9        | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 16       | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 17       | 0.91          |
| (2,900)  | 1:101:A:THR:CA | 1:102:A:PRO:CB | 18       | 0.91          |
| (2,839)  | 1:69:A:PHE:CB  | 1:31:A:PRO:CB  | 19       | 0.91          |
| (2,797)  | 1:126:A:LEU:CB | 1:127:A:PRO:CB | 12       | 0.91          |
| (2,776)  | 1:28:A:GLN:H   | 1:30:A:VAL:CB  | 3        | 0.91          |
| (2,776)  | 1:28:A:GLN:H   | 1:30:A:VAL:CB  | 8        | 0.91          |
| (2,776)  | 1:28:A:GLN:H   | 1:30:A:VAL:CB  | 18       | 0.91          |
| (2,752)  | 1:99:A:THR:H   | 1:101:A:THR:CB | 16       | 0.91          |
| (2,723)  | 1:86:A:LEU:H   | 1:45:A:TRP:CB  | 1        | 0.91          |
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB  | 5        | 0.91          |
| (2,593)  | 1:16:A:PHE:H   | 1:64:A:LEU:CB  | 19       | 0.91          |
| (2,285)  | 1:46:A:TYR:CB  | 1:68:A:TYR:CB  | 18       | 0.91          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 6        | 0.91          |
| (2,208)  | 1:126:A:LEU:CA | 1:127:A:PRO:CB | 18       | 0.91          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1271) | 1:128:A:GLN:HA   | 1:20:A:ARG:HG2  | 15       | 0.91          |
| (1,1163) | 1:113:A:GLN:HG3  | 1:110:A:PRO:HB2 | 17       | 0.91          |
| (1,1096) | 1:119:A:ARG:HG3  | 1:117:A:PRO:HG3 | 10       | 0.91          |
| (1,944)  | 1:70:A:TYR:HB2   | 1:76:A:PRO:HD3  | 14       | 0.91          |
| (1,770)  | 1:111:A:THR:HB   | 1:110:A:PRO:HG3 | 7        | 0.91          |
| (1,710)  | 1:47:A:ARG:HG2   | 1:67:A:TRP:HE1  | 16       | 0.91          |
| (1,363)  | 1:66:A:ARG:H     | 1:48:A:HIS:HB3  | 4        | 0.91          |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 9        | 0.91          |
| (2,1163) | 1:99:A:THR:H     | 1:42:A:LYS:CB   | 13       | 0.9           |
| (2,1153) | 1:93:A:ALA:H     | 1:30:A:VAL:CB   | 4        | 0.9           |
| (2,1153) | 1:93:A:ALA:H     | 1:30:A:VAL:CB   | 9        | 0.9           |
| (2,1147) | 1:101:A:THR:CB   | 1:102:A:PRO:CB  | 3        | 0.9           |
| (2,1147) | 1:101:A:THR:CB   | 1:102:A:PRO:CB  | 10       | 0.9           |
| (2,1147) | 1:101:A:THR:CB   | 1:102:A:PRO:CB  | 11       | 0.9           |
| (2,900)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 3        | 0.9           |
| (2,900)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 4        | 0.9           |
| (2,900)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 8        | 0.9           |
| (2,900)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 13       | 0.9           |
| (2,900)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 19       | 0.9           |
| (2,899)  | 1:110:A:PRO:CB   | 1:109:A:ASP:CA  | 7        | 0.9           |
| (2,839)  | 1:69:A:PHE:CB    | 1:31:A:PRO:CB   | 1        | 0.9           |
| (2,839)  | 1:69:A:PHE:CB    | 1:31:A:PRO:CB   | 18       | 0.9           |
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 2        | 0.9           |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 6        | 0.9           |
| (2,752)  | 1:99:A:THR:H     | 1:101:A:THR:CB  | 2        | 0.9           |
| (2,752)  | 1:99:A:THR:H     | 1:101:A:THR:CB  | 9        | 0.9           |
| (2,629)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 12       | 0.9           |
| (2,629)  | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 12       | 0.9           |
| (2,594)  | 1:29:A:GLY:H     | 1:92:A:VAL:CB   | 6        | 0.9           |
| (2,594)  | 1:29:A:GLY:H     | 1:92:A:VAL:CB   | 10       | 0.9           |
| (2,594)  | 1:29:A:GLY:H     | 1:92:A:VAL:CB   | 16       | 0.9           |
| (2,583)  | 1:105:A:VAL:CB   | 1:9:A:TRP:CB    | 5        | 0.9           |
| (2,582)  | 1:107:A:SER:CA   | 1:9:A:TRP:CB    | 8        | 0.9           |
| (2,565)  | 1:66:A:ARG:H     | 1:67:A:TRP:CB   | 16       | 0.9           |
| (2,537)  | 1:124:A:THR:H    | 1:28:A:GLN:CB   | 16       | 0.9           |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 6        | 0.9           |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 7        | 0.9           |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 11       | 0.9           |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 17       | 0.9           |
| (2,403)  | 1:105:A:VAL:H    | 1:74:A:THR:CB   | 16       | 0.9           |
| (2,379)  | 1:121:A:PRO:CA   | 1:32:A:ILE:CB   | 5        | 0.9           |
| (2,366)  | 1:120:A:PHE:CB   | 1:31:A:PRO:CB   | 7        | 0.9           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 10       | 0.9           |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 7        | 0.9           |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 7        | 0.9           |
| (2,239)  | 1:94:A:ASN:CB   | 1:96:A:GLN:CB   | 6        | 0.9           |
| (2,208)  | 1:126:A:LEU:CA  | 1:127:A:PRO:CB  | 17       | 0.9           |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 9        | 0.9           |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 9        | 0.9           |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 9        | 0.9           |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 4        | 0.9           |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 12       | 0.9           |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 18       | 0.9           |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 2        | 0.9           |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 10       | 0.9           |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3  | 16       | 0.9           |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 5        | 0.89          |
| (2,900)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 10       | 0.89          |
| (2,900)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 11       | 0.89          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 1        | 0.89          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 4        | 0.89          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 5        | 0.89          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 11       | 0.89          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 16       | 0.89          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 18       | 0.89          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 15       | 0.89          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 17       | 0.89          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 15       | 0.89          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 17       | 0.89          |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB   | 14       | 0.89          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 7        | 0.89          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 8        | 0.89          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 7        | 0.89          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 7        | 0.89          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 1        | 0.89          |
| (2,629)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 1        | 0.89          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB   | 7        | 0.89          |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 8        | 0.89          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 11       | 0.89          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 14       | 0.89          |
| (2,584)  | 1:108:A:ARG:CB  | 1:9:A:TRP:CB    | 1        | 0.89          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB   | 9        | 0.89          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB   | 18       | 0.89          |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 1        | 0.89          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 5        | 0.89          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 11       | 0.89          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 12       | 0.89          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 14       | 0.89          |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3  | 10       | 0.89          |
| (1,482)  | 1:104:A:ASP:HB3 | 1:36:A:VAL:HG23 | 19       | 0.89          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 11       | 0.89          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 13       | 0.89          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3  | 8        | 0.89          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 15       | 0.89          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 2        | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 5        | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 6        | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 7        | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 9        | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 14       | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 15       | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 16       | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 17       | 0.88          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 18       | 0.88          |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 17       | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 2        | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 3        | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 6        | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 8        | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 10       | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 13       | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 17       | 0.88          |
| (2,899)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 19       | 0.88          |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB  | 11       | 0.88          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 6        | 0.88          |
| (2,766)  | 1:120:A:PHE:CA  | 1:121:A:PRO:CB  | 18       | 0.88          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 5        | 0.88          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 6        | 0.88          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 15       | 0.88          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 17       | 0.88          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB  | 4        | 0.88          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 9        | 0.88          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 2        | 0.88          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 5        | 0.88          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 5        | 0.88          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 8        | 0.88          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,128)  | 1:28:A:GLN:CA    | 1:120:A:PHE:CB  | 18       | 0.88          |
| (1,1269) | 1:20:A:ARG:HG2   | 1:128:A:GLN:HG3 | 3        | 0.88          |
| (1,1163) | 1:113:A:GLN:HG3  | 1:110:A:PRO:HB2 | 16       | 0.88          |
| (1,840)  | 1:120:A:PHE:HA   | 1:32:A:ILE:HG12 | 3        | 0.88          |
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 2        | 0.88          |
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 7        | 0.88          |
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 14       | 0.88          |
| (1,482)  | 1:104:A:ASP:HB3  | 1:36:A:VAL:HG23 | 4        | 0.88          |
| (1,270)  | 1:112:A:THR:H    | 1:109:A:ASP:HB2 | 15       | 0.88          |
| (1,270)  | 1:112:A:THR:H    | 1:109:A:ASP:HB2 | 17       | 0.88          |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 3        | 0.88          |
| (1,104)  | 1:108:A:ARG:H    | 1:106:A:SER:HA  | 14       | 0.88          |
| (2,1163) | 1:99:A:THR:H     | 1:42:A:LYS:CB   | 11       | 0.87          |
| (2,1153) | 1:93:A:ALA:H     | 1:30:A:VAL:CB   | 8        | 0.87          |
| (2,1146) | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 3        | 0.87          |
| (2,1146) | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 4        | 0.87          |
| (2,1146) | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 8        | 0.87          |
| (2,1146) | 1:101:A:THR:CA   | 1:102:A:PRO:CB  | 13       | 0.87          |
| (2,1123) | 1:126:A:LEU:CB   | 1:13:A:ILE:CB   | 9        | 0.87          |
| (2,899)  | 1:110:A:PRO:CB   | 1:109:A:ASP:CA  | 12       | 0.87          |
| (2,899)  | 1:110:A:PRO:CB   | 1:109:A:ASP:CA  | 14       | 0.87          |
| (2,899)  | 1:110:A:PRO:CB   | 1:109:A:ASP:CA  | 15       | 0.87          |
| (2,889)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB   | 5        | 0.87          |
| (2,886)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB   | 2        | 0.87          |
| (2,867)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB   | 2        | 0.87          |
| (2,867)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB   | 5        | 0.87          |
| (2,867)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB   | 6        | 0.87          |
| (2,867)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB   | 16       | 0.87          |
| (2,860)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB   | 2        | 0.87          |
| (2,825)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB   | 5        | 0.87          |
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 8        | 0.87          |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 9        | 0.87          |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 10       | 0.87          |
| (2,766)  | 1:120:A:PHE:CA   | 1:121:A:PRO:CB  | 9        | 0.87          |
| (2,727)  | 1:114:A:GLU:CB   | 1:116:A:ILE:CB  | 1        | 0.87          |
| (2,537)  | 1:124:A:THR:H    | 1:28:A:GLN:CB   | 9        | 0.87          |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 1        | 0.87          |
| (2,226)  | 1:113:A:GLN:CB   | 1:9:A:TRP:CA    | 6        | 0.87          |
| (1,1163) | 1:113:A:GLN:HG3  | 1:110:A:PRO:HB2 | 1        | 0.87          |
| (1,1163) | 1:113:A:GLN:HG3  | 1:110:A:PRO:HB2 | 5        | 0.87          |
| (1,1162) | 1:62:A:GLN:HG2   | 1:63:A:LEU:HG   | 7        | 0.87          |
| (1,310)  | 1:46:A:TYR:HB2   | 1:68:A:TYR:HB2  | 3        | 0.87          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 2        | 0.87          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 17       | 0.86          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 18       | 0.86          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 10       | 0.86          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 11       | 0.86          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 19       | 0.86          |
| (2,900)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 1        | 0.86          |
| (2,900)  | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 12       | 0.86          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 2        | 0.86          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 6        | 0.86          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 16       | 0.86          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 14       | 0.86          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 2        | 0.86          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 6        | 0.86          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 16       | 0.86          |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB  | 5        | 0.86          |
| (2,651)  | 1:70:A:TYR:H    | 1:31:A:PRO:CB   | 18       | 0.86          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 13       | 0.86          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 9        | 0.86          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 17       | 0.86          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB   | 13       | 0.86          |
| (2,237)  | 1:24:A:PHE:H    | 1:90:A:PHE:CB   | 11       | 0.86          |
| (2,130)  | 1:120:A:PHE:CB  | 1:30:A:VAL:CA   | 8        | 0.86          |
| (2,81)   | 1:9:A:TRP:CB    | 1:71:A:TYR:CB   | 7        | 0.86          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 2        | 0.86          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 16       | 0.86          |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3  | 14       | 0.86          |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2 | 19       | 0.86          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 19       | 0.86          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 11       | 0.86          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 14       | 0.86          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 15       | 0.86          |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3  | 15       | 0.86          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 13       | 0.86          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 10       | 0.85          |
| (2,1202) | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 15       | 0.85          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 16       | 0.85          |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 14       | 0.85          |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 16       | 0.85          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 3        | 0.85          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 3        | 0.85          |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB  | 3        | 0.85          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 4        | 0.85          |
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 13       | 0.85          |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 13       | 0.85          |
| (2,727)  | 1:114:A:GLU:CB   | 1:116:A:ILE:CB  | 14       | 0.85          |
| (2,722)  | 1:114:A:GLU:CB   | 1:115:A:ALA:CB  | 5        | 0.85          |
| (2,594)  | 1:29:A:GLY:H     | 1:92:A:VAL:CB   | 4        | 0.85          |
| (2,587)  | 1:81:A:SER:CB    | 1:84:A:GLU:CB   | 3        | 0.85          |
| (2,587)  | 1:81:A:SER:CB    | 1:84:A:GLU:CB   | 5        | 0.85          |
| (2,105)  | 1:24:A:PHE:CA    | 1:125:A:ILE:CB  | 19       | 0.85          |
| (1,1253) | 1:122:A:PRO:HD3  | 1:121:A:PRO:HB2 | 10       | 0.85          |
| (1,1253) | 1:122:A:PRO:HD3  | 1:121:A:PRO:HB2 | 16       | 0.85          |
| (1,1253) | 1:122:A:PRO:HD3  | 1:121:A:PRO:HB2 | 17       | 0.85          |
| (1,1242) | 1:130:A:TYR:H    | 1:17:A:GLN:HB2  | 6        | 0.85          |
| (1,1162) | 1:62:A:GLN:HG2   | 1:63:A:LEU:HG   | 6        | 0.85          |
| (1,1005) | 1:135:A:SER:HA   | 1:117:A:PRO:HD2 | 2        | 0.85          |
| (1,840)  | 1:120:A:PHE:HA   | 1:32:A:ILE:HG12 | 13       | 0.85          |
| (1,789)  | 1:83:A:GLY:HA2   | 1:84:A:GLU:HG2  | 5        | 0.85          |
| (1,776)  | 1:125:A:ILE:H    | 1:25:A:SER:HB3  | 9        | 0.85          |
| (1,690)  | 1:99:A:THR:HA    | 1:42:A:LYS:HB3  | 18       | 0.85          |
| (1,346)  | 1:43:A:GLY:HA3   | 1:72:A:LEU:HA   | 1        | 0.85          |
| (1,346)  | 1:43:A:GLY:HA3   | 1:72:A:LEU:HA   | 3        | 0.85          |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 13       | 0.85          |
| (1,86)   | 1:101:A:THR:HB   | 1:100:A:SER:HB3 | 7        | 0.85          |
| (2,1153) | 1:93:A:ALA:H     | 1:30:A:VAL:CB   | 13       | 0.84          |
| (2,1123) | 1:126:A:LEU:CB   | 1:13:A:ILE:CB   | 18       | 0.84          |
| (2,899)  | 1:110:A:PRO:CB   | 1:109:A:ASP:CA  | 9        | 0.84          |
| (2,898)  | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 1        | 0.84          |
| (2,891)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB   | 6        | 0.84          |
| (2,888)  | 1:5:A:PRO:CB     | 1:6:A:HIS:CB    | 9        | 0.84          |
| (2,839)  | 1:69:A:PHE:CB    | 1:31:A:PRO:CB   | 7        | 0.84          |
| (2,839)  | 1:69:A:PHE:CB    | 1:31:A:PRO:CB   | 17       | 0.84          |
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 10       | 0.84          |
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 15       | 0.84          |
| (2,797)  | 1:126:A:LEU:CB   | 1:127:A:PRO:CB  | 16       | 0.84          |
| (2,723)  | 1:86:A:LEU:H     | 1:45:A:TRP:CB   | 15       | 0.84          |
| (2,587)  | 1:81:A:SER:CB    | 1:84:A:GLU:CB   | 8        | 0.84          |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 3        | 0.84          |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 10       | 0.84          |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 14       | 0.84          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 10       | 0.84          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 12       | 0.84          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 13       | 0.84          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 9        | 0.84          |
| (2,333)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 12       | 0.84          |
| (2,316)  | 1:36:A:VAL:H    | 1:37:A:PRO:CB   | 12       | 0.84          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 15       | 0.84          |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2 | 3        | 0.84          |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2 | 14       | 0.84          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 3        | 0.84          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 7        | 0.84          |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 5        | 0.84          |
| (1,377)  | 1:11:A:SER:H    | 1:10:A:PHE:HB2  | 17       | 0.84          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 16       | 0.84          |
| (1,86)   | 1:101:A:THR:HB  | 1:100:A:SER:HB3 | 2        | 0.84          |
| (1,86)   | 1:101:A:THR:HB  | 1:100:A:SER:HB3 | 9        | 0.84          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 10       | 0.83          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 1        | 0.83          |
| (2,1146) | 1:101:A:THR:CA  | 1:102:A:PRO:CB  | 12       | 0.83          |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 6        | 0.83          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 10       | 0.83          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 11       | 0.83          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 10       | 0.83          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 19       | 0.83          |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB  | 18       | 0.83          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB  | 8        | 0.83          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 17       | 0.83          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 6        | 0.83          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB   | 9        | 0.83          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 11       | 0.83          |
| (2,237)  | 1:24:A:PHE:H    | 1:90:A:PHE:CB   | 18       | 0.83          |
| (2,130)  | 1:120:A:PHE:CB  | 1:30:A:VAL:CA   | 9        | 0.83          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 1        | 0.83          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 11       | 0.83          |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 13       | 0.83          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 17       | 0.83          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 2        | 0.83          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 17       | 0.83          |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2 | 13       | 0.83          |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2 | 15       | 0.83          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 8        | 0.83          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 15       | 0.83          |
| (1,954)  | 1:14:A:THR:HA   | 1:66:A:ARG:HG2  | 17       | 0.83          |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 12       | 0.83          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 1        | 0.83          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,310)  | 1:46:A:TYR:HB2   | 1:68:A:TYR:HB2  | 9        | 0.83          |
| (1,86)   | 1:101:A:THR:HB   | 1:100:A:SER:HB3 | 15       | 0.83          |
| (2,1153) | 1:93:A:ALA:H     | 1:30:A:VAL:CB   | 2        | 0.82          |
| (2,961)  | 1:120:A:PHE:H    | 1:121:A:PRO:CB  | 6        | 0.82          |
| (2,898)  | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 4        | 0.82          |
| (2,898)  | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 6        | 0.82          |
| (2,898)  | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 17       | 0.82          |
| (2,897)  | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 11       | 0.82          |
| (2,886)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB   | 11       | 0.82          |
| (2,860)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB   | 11       | 0.82          |
| (2,783)  | 1:124:A:THR:CB   | 1:24:A:PHE:CB   | 1        | 0.82          |
| (2,776)  | 1:28:A:GLN:H     | 1:30:A:VAL:CB   | 17       | 0.82          |
| (2,722)  | 1:114:A:GLU:CB   | 1:115:A:ALA:CB  | 10       | 0.82          |
| (2,593)  | 1:16:A:PHE:H     | 1:64:A:LEU:CB   | 2        | 0.82          |
| (2,593)  | 1:16:A:PHE:H     | 1:64:A:LEU:CB   | 7        | 0.82          |
| (2,584)  | 1:108:A:ARG:CB   | 1:9:A:TRP:CB    | 9        | 0.82          |
| (2,444)  | 1:104:A:ASP:CB   | 1:36:A:VAL:CB   | 5        | 0.82          |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 12       | 0.82          |
| (2,370)  | 1:75:A:GLY:H     | 1:76:A:PRO:CB   | 5        | 0.82          |
| (2,283)  | 1:81:A:SER:CB    | 1:84:A:GLU:CB   | 2        | 0.82          |
| (2,188)  | 1:125:A:ILE:CB   | 1:23:A:LYS:CB   | 13       | 0.82          |
| (2,156)  | 1:4:A:ILE:CB     | 1:6:A:HIS:CB    | 2        | 0.82          |
| (2,102)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB   | 11       | 0.82          |
| (2,86)   | 1:4:A:ILE:CB     | 1:5:A:PRO:CB    | 2        | 0.82          |
| (2,56)   | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 1        | 0.82          |
| (1,1278) | 1:78:A:ALA:HA    | 1:76:A:PRO:HD3  | 18       | 0.82          |
| (1,1253) | 1:122:A:PRO:HD3  | 1:121:A:PRO:HB2 | 1        | 0.82          |
| (1,1253) | 1:122:A:PRO:HD3  | 1:121:A:PRO:HB2 | 2        | 0.82          |
| (1,1253) | 1:122:A:PRO:HD3  | 1:121:A:PRO:HB2 | 4        | 0.82          |
| (1,1253) | 1:122:A:PRO:HD3  | 1:121:A:PRO:HB2 | 11       | 0.82          |
| (1,1038) | 1:60:A:GLN:HB3   | 1:54:A:LYS:HE2  | 2        | 0.82          |
| (1,1038) | 1:60:A:GLN:HB3   | 1:54:A:LYS:HE3  | 2        | 0.82          |
| (1,1005) | 1:135:A:SER:HA   | 1:117:A:PRO:HD2 | 5        | 0.82          |
| (1,835)  | 1:89:A:VAL:HB    | 1:90:A:PHE:HB3  | 1        | 0.82          |
| (1,835)  | 1:89:A:VAL:HB    | 1:90:A:PHE:HB3  | 11       | 0.82          |
| (1,835)  | 1:89:A:VAL:HB    | 1:90:A:PHE:HB3  | 14       | 0.82          |
| (1,716)  | 1:68:A:TYR:H     | 1:46:A:TYR:HB2  | 13       | 0.82          |
| (1,310)  | 1:46:A:TYR:HB2   | 1:68:A:TYR:HB2  | 2        | 0.82          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3  | 7        | 0.82          |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 14       | 0.82          |
| (1,199)  | 1:125:A:ILE:HG12 | 1:126:A:LEU:HB2 | 15       | 0.82          |
| (1,86)   | 1:101:A:THR:HB   | 1:100:A:SER:HB3 | 16       | 0.82          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 7        | 0.81          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 13       | 0.81          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 18       | 0.81          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 18       | 0.81          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 6        | 0.81          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 6        | 0.81          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 15       | 0.81          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 9        | 0.81          |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB  | 15       | 0.81          |
| (2,676)  | 1:113:A:GLN:CB  | 1:112:A:THR:CB  | 15       | 0.81          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 18       | 0.81          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 1        | 0.81          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 12       | 0.81          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 10       | 0.81          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 19       | 0.81          |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 2        | 0.81          |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 14       | 0.81          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 3        | 0.81          |
| (1,1272) | 1:129:A:GLY:HA3 | 1:17:A:GLN:HB2  | 10       | 0.81          |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2 | 12       | 0.81          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG   | 11       | 0.81          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 3        | 0.81          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 15       | 0.81          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 4        | 0.81          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 1        | 0.81          |
| (1,86)   | 1:101:A:THR:HB  | 1:100:A:SER:HB3 | 6        | 0.81          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 16       | 0.81          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 15       | 0.8           |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB  | 15       | 0.8           |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 1        | 0.8           |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 15       | 0.8           |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 15       | 0.8           |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 8        | 0.8           |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 18       | 0.8           |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 19       | 0.8           |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 4        | 0.8           |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 19       | 0.8           |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 4        | 0.8           |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 9        | 0.8           |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 18       | 0.8           |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB  | 6        | 0.8           |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 10       | 0.8           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 18       | 0.8           |
| (2,604)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 12       | 0.8           |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 6        | 0.8           |
| (2,593)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB   | 1        | 0.8           |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 12       | 0.8           |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 10       | 0.8           |
| (2,417)  | 1:30:A:VAL:H    | 1:31:A:PRO:CB   | 12       | 0.8           |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 8        | 0.8           |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 7        | 0.8           |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 4        | 0.8           |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 6        | 0.8           |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 13       | 0.8           |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 17       | 0.8           |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 9        | 0.8           |
| (2,5)    | 1:44:A:TYR:H    | 1:91:A:TRP:CB   | 8        | 0.8           |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 4        | 0.8           |
| (1,1253) | 1:122:A:PRO:HD3 | 1:121:A:PRO:HB2 | 5        | 0.8           |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 12       | 0.8           |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 18       | 0.8           |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 14       | 0.8           |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 12       | 0.8           |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 6        | 0.8           |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 12       | 0.8           |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 16       | 0.8           |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 17       | 0.8           |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3  | 11       | 0.8           |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3  | 19       | 0.8           |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 5        | 0.8           |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 17       | 0.8           |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 8        | 0.8           |
| (1,86)   | 1:101:A:THR:HB  | 1:100:A:SER:HB3 | 17       | 0.8           |
| (1,86)   | 1:101:A:THR:HB  | 1:100:A:SER:HB3 | 18       | 0.8           |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 1        | 0.79          |
| (2,1123) | 1:126:A:LEU:CB  | 1:13:A:ILE:CB   | 8        | 0.79          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 18       | 0.79          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 5        | 0.79          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 7        | 0.79          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 8        | 0.79          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 14       | 0.79          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 15       | 0.79          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 16       | 0.79          |
| (2,897)  | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 5        | 0.79          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,888)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB     | 15       | 0.79          |
| (2,825)  | 1:76:A:PRO:CB  | 1:46:A:TYR:CB    | 19       | 0.79          |
| (2,670)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 7        | 0.79          |
| (2,584)  | 1:108:A:ARG:CB | 1:9:A:TRP:CB     | 15       | 0.79          |
| (2,564)  | 1:127:A:PRO:CB | 1:23:A:LYS:CB    | 13       | 0.79          |
| (2,379)  | 1:121:A:PRO:CA | 1:32:A:ILE:CB    | 15       | 0.79          |
| (2,366)  | 1:120:A:PHE:CB | 1:31:A:PRO:CB    | 19       | 0.79          |
| (2,358)  | 1:31:A:PRO:CB  | 1:10:A:PHE:CB    | 18       | 0.79          |
| (2,102)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB    | 17       | 0.79          |
| (1,1334) | 1:16:A:PHE:HB3 | 1:130:A:TYR:HB3  | 5        | 0.79          |
| (1,1278) | 1:78:A:ALA:HA  | 1:76:A:PRO:HD3   | 13       | 0.79          |
| (1,1269) | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3  | 6        | 0.79          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12  | 19       | 0.79          |
| (1,1038) | 1:60:A:GLN:HB3 | 1:54:A:LYS:HE2   | 7        | 0.79          |
| (1,1038) | 1:60:A:GLN:HB3 | 1:54:A:LYS:HE3   | 7        | 0.79          |
| (1,937)  | 1:69:A:PHE:HB2 | 1:31:A:PRO:HG2   | 14       | 0.79          |
| (1,835)  | 1:89:A:VAL:HB  | 1:90:A:PHE:HB3   | 15       | 0.79          |
| (1,835)  | 1:89:A:VAL:HB  | 1:90:A:PHE:HB3   | 19       | 0.79          |
| (1,780)  | 1:131:A:TYR:H  | 1:16:A:PHE:HB3   | 4        | 0.79          |
| (1,690)  | 1:99:A:THR:HA  | 1:42:A:LYS:HB3   | 5        | 0.79          |
| (1,270)  | 1:112:A:THR:H  | 1:109:A:ASP:HB2  | 3        | 0.79          |
| (1,86)   | 1:101:A:THR:HB | 1:100:A:SER:HB3  | 14       | 0.79          |
| (1,29)   | 1:126:A:LEU:HA | 1:125:A:ILE:HG12 | 13       | 0.79          |
| (2,1163) | 1:99:A:THR:H   | 1:42:A:LYS:CB    | 19       | 0.78          |
| (2,1102) | 1:130:A:TYR:H  | 1:17:A:GLN:CB    | 6        | 0.78          |
| (2,1086) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB    | 11       | 0.78          |
| (2,978)  | 1:65:A:PRO:CB  | 1:67:A:TRP:CB    | 15       | 0.78          |
| (2,939)  | 1:82:A:TYR:H   | 1:72:A:LEU:CB    | 19       | 0.78          |
| (2,898)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 3        | 0.78          |
| (2,898)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 11       | 0.78          |
| (2,898)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 12       | 0.78          |
| (2,898)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 18       | 0.78          |
| (2,888)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB     | 5        | 0.78          |
| (2,762)  | 1:126:A:LEU:H  | 1:127:A:PRO:CB   | 10       | 0.78          |
| (2,723)  | 1:86:A:LEU:H   | 1:45:A:TRP:CB    | 14       | 0.78          |
| (2,722)  | 1:114:A:GLU:CB | 1:115:A:ALA:CB   | 7        | 0.78          |
| (2,722)  | 1:114:A:GLU:CB | 1:115:A:ALA:CB   | 14       | 0.78          |
| (2,670)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 1        | 0.78          |
| (2,670)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 4        | 0.78          |
| (2,670)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 5        | 0.78          |
| (2,670)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 11       | 0.78          |
| (2,670)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 16       | 0.78          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 18       | 0.78          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 15       | 0.78          |
| (2,563)  | 1:42:A:LYS:H    | 1:71:A:TYR:CB   | 8        | 0.78          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 12       | 0.78          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 2        | 0.78          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 5        | 0.78          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB   | 11       | 0.78          |
| (2,285)  | 1:46:A:TYR:CB   | 1:68:A:TYR:CB   | 10       | 0.78          |
| (2,226)  | 1:113:A:GLN:CB  | 1:9:A:TRP:CA    | 16       | 0.78          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 14       | 0.78          |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 16       | 0.78          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 8        | 0.78          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 10       | 0.78          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 19       | 0.78          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 14       | 0.78          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 18       | 0.78          |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 10       | 0.78          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 10       | 0.78          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 12       | 0.78          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 18       | 0.78          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 16       | 0.78          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 14       | 0.78          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB  | 16       | 0.77          |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 7        | 0.77          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 1        | 0.77          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 6        | 0.77          |
| (2,961)  | 1:120:A:PHE:H   | 1:121:A:PRO:CB  | 9        | 0.77          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 9        | 0.77          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 8        | 0.77          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 18       | 0.77          |
| (2,853)  | 1:6:A:HIS:CB    | 1:4:A:ILE:CB    | 2        | 0.77          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 15       | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 2        | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 3        | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 6        | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 8        | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 10       | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 13       | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 17       | 0.77          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 19       | 0.77          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB   | 3        | 0.77          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 6        | 0.77          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 5        | 0.77          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 7        | 0.77          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 8        | 0.77          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 11       | 0.77          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 12       | 0.77          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 15       | 0.77          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 16       | 0.77          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 18       | 0.77          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 9        | 0.77          |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 18       | 0.77          |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 4        | 0.77          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 7        | 0.77          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 1        | 0.77          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 9        | 0.77          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2  | 3        | 0.77          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 10       | 0.77          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 7        | 0.77          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 9        | 0.77          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 16       | 0.77          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 7        | 0.77          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 14       | 0.77          |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2  | 9        | 0.77          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 11       | 0.76          |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 19       | 0.76          |
| (2,1019) | 1:38:A:PRO:CB   | 1:96:A:GLN:CB   | 19       | 0.76          |
| (2,889)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 10       | 0.76          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 12       | 0.76          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 14       | 0.76          |
| (2,867)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 10       | 0.76          |
| (2,825)  | 1:76:A:PRO:CB   | 1:46:A:TYR:CB   | 10       | 0.76          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 12       | 0.76          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 14       | 0.76          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 15       | 0.76          |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 9        | 0.76          |
| (2,537)  | 1:124:A:THR:H   | 1:28:A:GLN:CB   | 11       | 0.76          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 4        | 0.76          |
| (2,130)  | 1:120:A:PHE:CB  | 1:30:A:VAL:CA   | 18       | 0.76          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 3        | 0.76          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 9        | 0.76          |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 15       | 0.76          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 5        | 0.76          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 12       | 0.76          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 10       | 0.76          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 13       | 0.76          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 10       | 0.76          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 15       | 0.76          |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 19       | 0.76          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 8        | 0.76          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 3        | 0.76          |
| (1,363)  | 1:66:A:ARG:H    | 1:48:A:HIS:HB3  | 2        | 0.76          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 7        | 0.76          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 5        | 0.76          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 12       | 0.76          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 19       | 0.76          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB  | 6        | 0.75          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB  | 14       | 0.75          |
| (2,1139) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 12       | 0.75          |
| (2,1065) | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 12       | 0.75          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 1        | 0.75          |
| (2,920)  | 1:9:A:TRP:CB    | 1:108:A:ARG:CB  | 12       | 0.75          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 7        | 0.75          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 12       | 0.75          |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB  | 3        | 0.75          |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB  | 8        | 0.75          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 17       | 0.75          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 10       | 0.75          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 3        | 0.75          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 13       | 0.75          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB   | 17       | 0.75          |
| (2,10)   | 1:116:A:ILE:CB  | 1:117:A:PRO:CB  | 17       | 0.75          |
| (1,1363) | 1:52:A:SER:HB2  | 1:62:A:GLN:HG2  | 12       | 0.75          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3  | 11       | 0.75          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 4        | 0.75          |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 2        | 0.75          |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 4        | 0.75          |
| (1,835)  | 1:89:A:VAL:HB   | 1:90:A:PHE:HB3  | 9        | 0.75          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3  | 17       | 0.75          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 11       | 0.75          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 15       | 0.75          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 6        | 0.75          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 6        | 0.75          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 17       | 0.75          |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 1        | 0.75          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB   | 1        | 0.74          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB   | 18       | 0.74          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 3        | 0.74          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 11       | 0.74          |
| (2,888)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 16       | 0.74          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB   | 13       | 0.74          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB    | 17       | 0.74          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 1        | 0.74          |
| (2,152)  | 1:7:A:TYR:CB    | 1:110:A:PRO:CB   | 7        | 0.74          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB   | 6        | 0.74          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB   | 13       | 0.74          |
| (2,68)   | 1:86:A:LEU:H    | 1:45:A:TRP:CB    | 2        | 0.74          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3  | 1        | 0.74          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3  | 19       | 0.74          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3   | 13       | 0.74          |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12  | 3        | 0.74          |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12  | 6        | 0.74          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2  | 18       | 0.74          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 4        | 0.74          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 10       | 0.74          |
| (1,288)  | 1:16:A:PHE:HA   | 1:64:A:LEU:HD23  | 1        | 0.74          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2  | 18       | 0.74          |
| (1,29)   | 1:126:A:LEU:HA  | 1:125:A:ILE:HG12 | 1        | 0.74          |
| (2,1153) | 1:93:A:ALA:H    | 1:30:A:VAL:CB    | 3        | 0.73          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB   | 7        | 0.73          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB   | 17       | 0.73          |
| (2,958)  | 1:64:A:LEU:H    | 1:65:A:PRO:CB    | 5        | 0.73          |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB    | 16       | 0.73          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB    | 19       | 0.73          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB    | 19       | 0.73          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB   | 12       | 0.73          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB   | 10       | 0.73          |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB   | 11       | 0.73          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB     | 6        | 0.73          |
| (2,670)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA   | 9        | 0.73          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 15       | 0.73          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB    | 8        | 0.73          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB    | 14       | 0.73          |
| (2,370)  | 1:75:A:GLY:H    | 1:76:A:PRO:CB    | 1        | 0.73          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB    | 19       | 0.73          |
| (2,240)  | 1:20:A:ARG:H    | 1:17:A:GLN:CB    | 1        | 0.73          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 9        | 0.73          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 18       | 0.73          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,188)  | 1:125:A:ILE:CB  | 1:23:A:LYS:CB    | 3        | 0.73          |
| (2,156)  | 1:4:A:ILE:CB    | 1:6:A:HIS:CB     | 1        | 0.73          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB   | 3        | 0.73          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3   | 7        | 0.73          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3   | 16       | 0.73          |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12  | 13       | 0.73          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2  | 15       | 0.73          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2  | 11       | 0.73          |
| (1,910)  | 1:94:A:ASN:HB3  | 1:27:A:GLY:HA2   | 18       | 0.73          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3   | 5        | 0.73          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3   | 12       | 0.73          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3   | 17       | 0.73          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12  | 2        | 0.73          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 1        | 0.73          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 2        | 0.73          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 3        | 0.73          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 17       | 0.73          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 18       | 0.73          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3   | 1        | 0.73          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3   | 5        | 0.73          |
| (1,29)   | 1:126:A:LEU:HA  | 1:125:A:ILE:HG12 | 15       | 0.73          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB   | 1        | 0.72          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB   | 12       | 0.72          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB    | 12       | 0.72          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB    | 18       | 0.72          |
| (2,897)  | 1:64:A:LEU:CB   | 1:65:A:PRO:CB    | 4        | 0.72          |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB   | 9        | 0.72          |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB   | 14       | 0.72          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 19       | 0.72          |
| (2,565)  | 1:66:A:ARG:H    | 1:67:A:TRP:CB    | 9        | 0.72          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB    | 1        | 0.72          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 11       | 0.72          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 14       | 0.72          |
| (2,237)  | 1:24:A:PHE:H    | 1:90:A:PHE:CB    | 10       | 0.72          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 4        | 0.72          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 6        | 0.72          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 7        | 0.72          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 8        | 0.72          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 12       | 0.72          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 16       | 0.72          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 19       | 0.72          |
| (1,1278) | 1:78:A:ALA:HA   | 1:76:A:PRO:HD3   | 1        | 0.72          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1216) | 1:100:A:SER:H   | 1:42:A:LYS:HE3  | 14       | 0.72          |
| (1,1216) | 1:100:A:SER:H   | 1:42:A:LYS:HE3  | 17       | 0.72          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 11       | 0.72          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 4        | 0.72          |
| (1,844)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE21 | 7        | 0.72          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 17       | 0.72          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 11       | 0.72          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 7        | 0.72          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 9        | 0.72          |
| (2,1147) | 1:101:A:THR:CB  | 1:102:A:PRO:CB  | 9        | 0.71          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 19       | 0.71          |
| (2,897)  | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 3        | 0.71          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 9        | 0.71          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 9        | 0.71          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 4        | 0.71          |
| (2,839)  | 1:69:A:PHE:CB   | 1:31:A:PRO:CB   | 16       | 0.71          |
| (2,797)  | 1:126:A:LEU:CB  | 1:127:A:PRO:CB  | 19       | 0.71          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 13       | 0.71          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 10       | 0.71          |
| (2,752)  | 1:99:A:THR:H    | 1:101:A:THR:CB  | 4        | 0.71          |
| (2,723)  | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 5        | 0.71          |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB  | 9        | 0.71          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 3        | 0.71          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 18       | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 1        | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 2        | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 3        | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 10       | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 13       | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 14       | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 15       | 0.71          |
| (2,192)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 17       | 0.71          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB   | 2        | 0.71          |
| (2,10)   | 1:116:A:ILE:CB  | 1:117:A:PRO:CB  | 12       | 0.71          |
| (2,10)   | 1:116:A:ILE:CB  | 1:117:A:PRO:CB  | 19       | 0.71          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 2        | 0.71          |
| (1,1216) | 1:100:A:SER:H   | 1:42:A:LYS:HE3  | 2        | 0.71          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 1        | 0.71          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 19       | 0.71          |
| (1,785)  | 1:113:A:GLN:HG2 | 1:110:A:PRO:HB2 | 6        | 0.71          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3  | 2        | 0.71          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3  | 14       | 0.71          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,776)  | 1:125:A:ILE:H  | 1:25:A:SER:HB3  | 2        | 0.71          |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2  | 5        | 0.71          |
| (1,710)  | 1:47:A:ARG:HG2 | 1:67:A:TRP:HE1  | 3        | 0.71          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23 | 2        | 0.71          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 13       | 0.71          |
| (2,1153) | 1:93:A:ALA:H   | 1:30:A:VAL:CB   | 19       | 0.7           |
| (2,1147) | 1:101:A:THR:CB | 1:102:A:PRO:CB  | 2        | 0.7           |
| (2,1147) | 1:101:A:THR:CB | 1:102:A:PRO:CB  | 5        | 0.7           |
| (2,1124) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB   | 4        | 0.7           |
| (2,1123) | 1:126:A:LEU:CB | 1:13:A:ILE:CB   | 19       | 0.7           |
| (2,1044) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB   | 4        | 0.7           |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 8        | 0.7           |
| (2,889)  | 1:76:A:PRO:CB  | 1:46:A:TYR:CB   | 4        | 0.7           |
| (2,888)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB    | 6        | 0.7           |
| (2,888)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB    | 13       | 0.7           |
| (2,867)  | 1:76:A:PRO:CB  | 1:46:A:TYR:CB   | 4        | 0.7           |
| (2,854)  | 1:14:A:THR:CA  | 1:66:A:ARG:CB   | 10       | 0.7           |
| (2,797)  | 1:126:A:LEU:CB | 1:127:A:PRO:CB  | 7        | 0.7           |
| (2,762)  | 1:126:A:LEU:H  | 1:127:A:PRO:CB  | 3        | 0.7           |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB  | 8        | 0.7           |
| (2,593)  | 1:16:A:PHE:H   | 1:64:A:LEU:CB   | 12       | 0.7           |
| (2,582)  | 1:107:A:SER:CA | 1:9:A:TRP:CB    | 19       | 0.7           |
| (2,324)  | 1:63:A:LEU:H   | 1:52:A:SER:CB   | 3        | 0.7           |
| (2,192)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 11       | 0.7           |
| (2,84)   | 1:44:A:TYR:CB  | 1:91:A:TRP:CB   | 7        | 0.7           |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 2        | 0.7           |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 9        | 0.7           |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 13       | 0.7           |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 14       | 0.7           |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 18       | 0.7           |
| (1,1269) | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 17       | 0.7           |
| (1,1269) | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 19       | 0.7           |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12 | 11       | 0.7           |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12 | 17       | 0.7           |
| (1,1216) | 1:100:A:SER:H  | 1:42:A:LYS:HE3  | 16       | 0.7           |
| (1,1206) | 1:135:A:SER:HA | 1:117:A:PRO:HG2 | 8        | 0.7           |
| (1,955)  | 1:13:A:ILE:HA  | 1:66:A:ARG:HG2  | 19       | 0.7           |
| (1,888)  | 1:20:A:ARG:HD2 | 1:128:A:GLN:HG3 | 17       | 0.7           |
| (1,780)  | 1:131:A:TYR:H  | 1:16:A:PHE:HB3  | 6        | 0.7           |
| (1,690)  | 1:99:A:THR:HA  | 1:42:A:LYS:HB3  | 12       | 0.7           |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2  | 16       | 0.7           |
| (1,346)  | 1:43:A:GLY:HA3 | 1:72:A:LEU:HA   | 14       | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,277)  | 1:111:A:THR:H    | 1:110:A:PRO:HB3  | 2        | 0.7           |
| (1,277)  | 1:111:A:THR:H    | 1:110:A:PRO:HB3  | 12       | 0.7           |
| (1,277)  | 1:111:A:THR:H    | 1:110:A:PRO:HB3  | 17       | 0.7           |
| (1,270)  | 1:112:A:THR:H    | 1:109:A:ASP:HB2  | 10       | 0.7           |
| (1,29)   | 1:126:A:LEU:HA   | 1:125:A:ILE:HG12 | 14       | 0.7           |
| (1,24)   | 1:128:A:GLN:HE21 | 1:20:A:ARG:HD2   | 4        | 0.7           |
| (2,1201) | 1:52:A:SER:CB    | 1:62:A:GLN:CB    | 12       | 0.69          |
| (2,978)  | 1:65:A:PRO:CB    | 1:67:A:TRP:CB    | 13       | 0.69          |
| (2,891)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB    | 7        | 0.69          |
| (2,888)  | 1:5:A:PRO:CB     | 1:6:A:HIS:CB     | 17       | 0.69          |
| (2,886)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB    | 16       | 0.69          |
| (2,860)  | 1:130:A:TYR:CB   | 1:20:A:ARG:CB    | 16       | 0.69          |
| (2,853)  | 1:6:A:HIS:CB     | 1:4:A:ILE:CB     | 1        | 0.69          |
| (2,825)  | 1:76:A:PRO:CB    | 1:46:A:TYR:CB    | 4        | 0.69          |
| (2,762)  | 1:126:A:LEU:H    | 1:127:A:PRO:CB   | 8        | 0.69          |
| (2,727)  | 1:114:A:GLU:CB   | 1:116:A:ILE:CB   | 3        | 0.69          |
| (2,721)  | 1:45:A:TRP:H     | 1:89:A:VAL:CB    | 16       | 0.69          |
| (2,676)  | 1:113:A:GLN:CB   | 1:112:A:THR:CB   | 6        | 0.69          |
| (2,676)  | 1:113:A:GLN:CB   | 1:112:A:THR:CB   | 7        | 0.69          |
| (2,676)  | 1:113:A:GLN:CB   | 1:112:A:THR:CB   | 10       | 0.69          |
| (2,564)  | 1:127:A:PRO:CB   | 1:23:A:LYS:CB    | 10       | 0.69          |
| (2,283)  | 1:81:A:SER:CB    | 1:84:A:GLU:CB    | 9        | 0.69          |
| (2,192)  | 1:30:A:VAL:CA    | 1:31:A:PRO:CB    | 5        | 0.69          |
| (2,179)  | 1:103:A:SER:H    | 1:72:A:LEU:CB    | 18       | 0.69          |
| (2,130)  | 1:120:A:PHE:CB   | 1:30:A:VAL:CA    | 7        | 0.69          |
| (2,21)   | 1:128:A:GLN:CB   | 1:20:A:ARG:CB    | 10       | 0.69          |
| (2,10)   | 1:116:A:ILE:CB   | 1:117:A:PRO:CB   | 6        | 0.69          |
| (2,10)   | 1:116:A:ILE:CB   | 1:117:A:PRO:CB   | 10       | 0.69          |
| (1,1161) | 1:62:A:GLN:HG2   | 1:63:A:LEU:HB3   | 14       | 0.69          |
| (1,1128) | 1:73:A:GLY:HA3   | 1:102:A:PRO:HG2  | 7        | 0.69          |
| (1,1121) | 1:130:A:TYR:H    | 1:127:A:PRO:HG3  | 14       | 0.69          |
| (1,1005) | 1:135:A:SER:HA   | 1:117:A:PRO:HD2  | 9        | 0.69          |
| (1,851)  | 1:28:A:GLN:H     | 1:25:A:SER:HB3   | 9        | 0.69          |
| (1,780)  | 1:131:A:TYR:H    | 1:16:A:PHE:HB3   | 18       | 0.69          |
| (1,716)  | 1:68:A:TYR:H     | 1:46:A:TYR:HB2   | 4        | 0.69          |
| (1,388)  | 1:104:A:ASP:H    | 1:40:A:GLU:HB2   | 5        | 0.69          |
| (1,310)  | 1:46:A:TYR:HB2   | 1:68:A:TYR:HB2   | 1        | 0.69          |
| (1,286)  | 1:16:A:PHE:HA    | 1:64:A:LEU:HD22  | 15       | 0.69          |
| (1,277)  | 1:111:A:THR:H    | 1:110:A:PRO:HB3  | 9        | 0.69          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3   | 1        | 0.69          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3   | 15       | 0.69          |
| (1,54)   | 1:63:A:LEU:HA    | 1:62:A:GLN:HG2   | 8        | 0.69          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,1086) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB   | 16       | 0.68          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 2        | 0.68          |
| (2,888)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB    | 4        | 0.68          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 7        | 0.68          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 10       | 0.68          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 13       | 0.68          |
| (2,797)  | 1:126:A:LEU:CB | 1:127:A:PRO:CB  | 1        | 0.68          |
| (2,783)  | 1:124:A:THR:CB | 1:24:A:PHE:CB   | 14       | 0.68          |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB   | 4        | 0.68          |
| (2,752)  | 1:99:A:THR:H   | 1:101:A:THR:CB  | 1        | 0.68          |
| (2,366)  | 1:120:A:PHE:CB | 1:31:A:PRO:CB   | 16       | 0.68          |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB   | 3        | 0.68          |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB   | 5        | 0.68          |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB   | 7        | 0.68          |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB   | 9        | 0.68          |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 1        | 0.68          |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 3        | 0.68          |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 4        | 0.68          |
| (2,9)    | 1:4:A:ILE:CB   | 1:6:A:HIS:CB    | 5        | 0.68          |
| (2,9)    | 1:4:A:ILE:CB   | 1:6:A:HIS:CB    | 15       | 0.68          |
| (2,3)    | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 8        | 0.68          |
| (1,1363) | 1:52:A:SER:HB2 | 1:62:A:GLN:HG2  | 10       | 0.68          |
| (1,1269) | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3 | 16       | 0.68          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12 | 12       | 0.68          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12 | 14       | 0.68          |
| (1,1216) | 1:100:A:SER:H  | 1:42:A:LYS:HE3  | 7        | 0.68          |
| (1,1161) | 1:62:A:GLN:HG2 | 1:63:A:LEU:HB3  | 10       | 0.68          |
| (1,1128) | 1:73:A:GLY:HA3 | 1:102:A:PRO:HG2 | 2        | 0.68          |
| (1,840)  | 1:120:A:PHE:HA | 1:32:A:ILE:HG12 | 1        | 0.68          |
| (1,835)  | 1:89:A:VAL:HB  | 1:90:A:PHE:HB3  | 13       | 0.68          |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2  | 3        | 0.68          |
| (1,789)  | 1:83:A:GLY:HA2 | 1:84:A:GLU:HG2  | 8        | 0.68          |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2  | 11       | 0.68          |
| (1,710)  | 1:47:A:ARG:HG2 | 1:67:A:TRP:HE1  | 7        | 0.68          |
| (1,654)  | 1:16:A:PHE:H   | 1:64:A:LEU:HD23 | 15       | 0.68          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23 | 4        | 0.68          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23 | 15       | 0.68          |
| (1,310)  | 1:46:A:TYR:HB2 | 1:68:A:TYR:HB2  | 8        | 0.68          |
| (1,310)  | 1:46:A:TYR:HB2 | 1:68:A:TYR:HB2  | 11       | 0.68          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 3        | 0.68          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 8        | 0.68          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 15       | 0.68          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,270)  | 1:112:A:THR:H  | 1:109:A:ASP:HB2 | 16       | 0.68          |
| (2,891)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 2        | 0.67          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB  | 9        | 0.67          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB  | 11       | 0.67          |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB   | 8        | 0.67          |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB   | 17       | 0.67          |
| (2,102)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 6        | 0.67          |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 15       | 0.67          |
| (1,1216) | 1:100:A:SER:H  | 1:42:A:LYS:HE3  | 15       | 0.67          |
| (1,944)  | 1:70:A:TYR:HB2 | 1:76:A:PRO:HD3  | 9        | 0.67          |
| (1,851)  | 1:28:A:GLN:H   | 1:25:A:SER:HB3  | 11       | 0.67          |
| (1,835)  | 1:89:A:VAL:HB  | 1:90:A:PHE:HB3  | 7        | 0.67          |
| (1,835)  | 1:89:A:VAL:HB  | 1:90:A:PHE:HB3  | 8        | 0.67          |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2  | 1        | 0.67          |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2  | 2        | 0.67          |
| (2,978)  | 1:65:A:PRO:CB  | 1:67:A:TRP:CB   | 7        | 0.66          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 6        | 0.66          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 14       | 0.66          |
| (2,888)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB    | 19       | 0.66          |
| (2,886)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 7        | 0.66          |
| (2,860)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 7        | 0.66          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 2        | 0.66          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB   | 5        | 0.66          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB   | 6        | 0.66          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 6        | 0.66          |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB   | 6        | 0.66          |
| (2,762)  | 1:126:A:LEU:H  | 1:127:A:PRO:CB  | 18       | 0.66          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB   | 9        | 0.66          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB   | 13       | 0.66          |
| (2,722)  | 1:114:A:GLU:CB | 1:115:A:ALA:CB  | 6        | 0.66          |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB   | 2        | 0.66          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB  | 4        | 0.66          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 3        | 0.66          |
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB   | 3        | 0.66          |
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB   | 13       | 0.66          |
| (2,565)  | 1:66:A:ARG:H   | 1:67:A:TRP:CB   | 3        | 0.66          |
| (2,564)  | 1:127:A:PRO:CB | 1:23:A:LYS:CB   | 3        | 0.66          |
| (2,379)  | 1:121:A:PRO:CA | 1:32:A:ILE:CB   | 13       | 0.66          |
| (2,358)  | 1:31:A:PRO:CB  | 1:10:A:PHE:CB   | 14       | 0.66          |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB   | 17       | 0.66          |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB   | 16       | 0.66          |
| (2,105)  | 1:24:A:PHE:CA  | 1:125:A:ILE:CB  | 10       | 0.66          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,10)   | 1:116:A:ILE:CB  | 1:117:A:PRO:CB   | 7        | 0.66          |
| (2,10)   | 1:116:A:ILE:CB  | 1:117:A:PRO:CB   | 11       | 0.66          |
| (2,10)   | 1:116:A:ILE:CB  | 1:117:A:PRO:CB   | 16       | 0.66          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3   | 18       | 0.66          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2  | 4        | 0.66          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2  | 10       | 0.66          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2  | 13       | 0.66          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2   | 11       | 0.66          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3   | 7        | 0.66          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1   | 1        | 0.66          |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3   | 4        | 0.66          |
| (1,277)  | 1:111:A:THR:H   | 1:110:A:PRO:HB3  | 10       | 0.66          |
| (1,277)  | 1:111:A:THR:H   | 1:110:A:PRO:HB3  | 19       | 0.66          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 12       | 0.66          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2   | 4        | 0.66          |
| (1,29)   | 1:126:A:LEU:HA  | 1:125:A:ILE:HG12 | 3        | 0.66          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB    | 5        | 0.65          |
| (2,954)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA     | 2        | 0.65          |
| (2,954)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CA     | 2        | 0.65          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB   | 19       | 0.65          |
| (2,838)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB     | 1        | 0.65          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 11       | 0.65          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 11       | 0.65          |
| (2,778)  | 1:29:A:GLY:H    | 1:120:A:PHE:CB   | 18       | 0.65          |
| (2,614)  | 1:41:A:ALA:H    | 1:36:A:VAL:CB    | 12       | 0.65          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB     | 14       | 0.65          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB    | 15       | 0.65          |
| (2,221)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 6        | 0.65          |
| (2,221)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 8        | 0.65          |
| (2,221)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 9        | 0.65          |
| (2,221)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB    | 18       | 0.65          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB    | 3        | 0.65          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB    | 14       | 0.65          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB    | 15       | 0.65          |
| (2,156)  | 1:4:A:ILE:CB    | 1:6:A:HIS:CB     | 10       | 0.65          |
| (2,130)  | 1:120:A:PHE:CB  | 1:30:A:VAL:CA    | 6        | 0.65          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3  | 4        | 0.65          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3   | 6        | 0.65          |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12  | 1        | 0.65          |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12  | 15       | 0.65          |
| (1,1162) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HG    | 1        | 0.65          |
| (1,1121) | 1:130:A:TYR:H   | 1:127:A:PRO:HG3  | 13       | 0.65          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1103) | 1:55:A:THR:H   | 1:54:A:LYS:HD3   | 18       | 0.65          |
| (1,851)  | 1:28:A:GLN:H   | 1:25:A:SER:HB3   | 16       | 0.65          |
| (1,835)  | 1:89:A:VAL:HB  | 1:90:A:PHE:HB3   | 3        | 0.65          |
| (1,710)  | 1:47:A:ARG:HG2 | 1:67:A:TRP:HE1   | 15       | 0.65          |
| (1,380)  | 1:31:A:PRO:HA  | 1:32:A:ILE:HG12  | 2        | 0.65          |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2   | 15       | 0.65          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3  | 1        | 0.65          |
| (1,42)   | 1:63:A:LEU:HA  | 1:52:A:SER:HB2   | 17       | 0.65          |
| (1,29)   | 1:126:A:LEU:HA | 1:125:A:ILE:HG12 | 9        | 0.65          |
| (2,1123) | 1:126:A:LEU:CB | 1:13:A:ILE:CB    | 7        | 0.64          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB    | 9        | 0.64          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB    | 13       | 0.64          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB    | 19       | 0.64          |
| (2,891)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB    | 1        | 0.64          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB   | 3        | 0.64          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB   | 11       | 0.64          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB   | 16       | 0.64          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 10       | 0.64          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 19       | 0.64          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB    | 2        | 0.64          |
| (2,722)  | 1:114:A:GLU:CB | 1:115:A:ALA:CB   | 4        | 0.64          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB   | 1        | 0.64          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB   | 5        | 0.64          |
| (2,458)  | 1:93:A:ALA:H   | 1:27:A:GLY:H     | 18       | 0.64          |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB    | 18       | 0.64          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB    | 4        | 0.64          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB    | 7        | 0.64          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB    | 12       | 0.64          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB    | 15       | 0.64          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB    | 16       | 0.64          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB    | 17       | 0.64          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB    | 19       | 0.64          |
| (2,9)    | 1:4:A:ILE:CB   | 1:6:A:HIS:CB     | 18       | 0.64          |
| (1,1278) | 1:78:A:ALA:HA  | 1:76:A:PRO:HD3   | 6        | 0.64          |
| (1,1216) | 1:100:A:SER:H  | 1:42:A:LYS:HE3   | 4        | 0.64          |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2   | 10       | 0.64          |
| (1,642)  | 1:10:A:PHE:H   | 1:9:A:TRP:HZ3    | 7        | 0.64          |
| (1,498)  | 1:93:A:ALA:H   | 1:27:A:GLY:H     | 18       | 0.64          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2   | 15       | 0.64          |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3   | 11       | 0.64          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3  | 4        | 0.64          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3  | 5        | 0.64          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 11       | 0.64          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 14       | 0.64          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 16       | 0.64          |
| (1,270)  | 1:112:A:THR:H  | 1:109:A:ASP:HB2 | 4        | 0.64          |
| (2,1102) | 1:130:A:TYR:H  | 1:17:A:GLN:CB   | 2        | 0.63          |
| (2,1102) | 1:130:A:TYR:H  | 1:17:A:GLN:CB   | 4        | 0.63          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 6        | 0.63          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 6        | 0.63          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 13       | 0.63          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 13       | 0.63          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 7        | 0.63          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 12       | 0.63          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 17       | 0.63          |
| (2,886)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 13       | 0.63          |
| (2,860)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 13       | 0.63          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB    | 4        | 0.63          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB    | 6        | 0.63          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB    | 17       | 0.63          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 7        | 0.63          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 9        | 0.63          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 18       | 0.63          |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB   | 17       | 0.63          |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB  | 6        | 0.63          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB  | 8        | 0.63          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 8        | 0.63          |
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB   | 14       | 0.63          |
| (2,594)  | 1:29:A:GLY:H   | 1:92:A:VAL:CB   | 7        | 0.63          |
| (2,369)  | 1:96:A:GLN:CB  | 1:38:A:PRO:CB   | 18       | 0.63          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 1        | 0.63          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 2        | 0.63          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 3        | 0.63          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 10       | 0.63          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 11       | 0.63          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 13       | 0.63          |
| (2,221)  | 1:30:A:VAL:CA  | 1:31:A:PRO:CB   | 14       | 0.63          |
| (2,10)   | 1:116:A:ILE:CB | 1:117:A:PRO:CB  | 5        | 0.63          |
| (2,3)    | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 11       | 0.63          |
| (1,1242) | 1:130:A:TYR:H  | 1:17:A:GLN:HB2  | 8        | 0.63          |
| (1,1242) | 1:130:A:TYR:H  | 1:17:A:GLN:HB2  | 19       | 0.63          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12 | 10       | 0.63          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12 | 16       | 0.63          |
| (1,1216) | 1:100:A:SER:H  | 1:42:A:LYS:HE3  | 5        | 0.63          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1140) | 1:50:A:ARG:HB3 | 1:66:A:ARG:HD2  | 3        | 0.63          |
| (1,1140) | 1:50:A:ARG:HB2 | 1:66:A:ARG:HD2  | 3        | 0.63          |
| (1,840)  | 1:120:A:PHE:HA | 1:32:A:ILE:HG12 | 5        | 0.63          |
| (1,840)  | 1:120:A:PHE:HA | 1:32:A:ILE:HG12 | 16       | 0.63          |
| (1,789)  | 1:83:A:GLY:HA2 | 1:84:A:GLU:HG2  | 19       | 0.63          |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2  | 10       | 0.63          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2  | 9        | 0.63          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2  | 18       | 0.63          |
| (1,349)  | 1:63:A:LEU:H   | 1:52:A:SER:HB2  | 1        | 0.63          |
| (1,310)  | 1:46:A:TYR:HB2 | 1:68:A:TYR:HB2  | 18       | 0.63          |
| (1,42)   | 1:63:A:LEU:HA  | 1:52:A:SER:HB2  | 11       | 0.63          |
| (2,1102) | 1:130:A:TYR:H  | 1:17:A:GLN:CB   | 11       | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 4        | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 4        | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 10       | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 10       | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 17       | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 17       | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 19       | 0.62          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 19       | 0.62          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB   | 18       | 0.62          |
| (2,886)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 18       | 0.62          |
| (2,860)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB   | 18       | 0.62          |
| (2,839)  | 1:69:A:PHE:CB  | 1:31:A:PRO:CB   | 8        | 0.62          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB    | 13       | 0.62          |
| (2,792)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB    | 13       | 0.62          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 8        | 0.62          |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB   | 7        | 0.62          |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB  | 1        | 0.62          |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB  | 16       | 0.62          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 6        | 0.62          |
| (2,571)  | 1:89:A:VAL:CB  | 1:45:A:TRP:CB   | 2        | 0.62          |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB   | 18       | 0.62          |
| (2,396)  | 1:15:A:GLN:H   | 1:64:A:LEU:CB   | 5        | 0.62          |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB   | 12       | 0.62          |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA  | 7        | 0.62          |
| (1,1154) | 1:11:A:SER:HA  | 1:136:A:GLY:HA3 | 9        | 0.62          |
| (1,1154) | 1:11:A:SER:HA  | 1:136:A:GLY:HA3 | 14       | 0.62          |
| (1,1121) | 1:130:A:TYR:H  | 1:127:A:PRO:HG3 | 10       | 0.62          |
| (1,1103) | 1:55:A:THR:H   | 1:54:A:LYS:HD3  | 17       | 0.62          |
| (1,851)  | 1:28:A:GLN:H   | 1:25:A:SER:HB3  | 6        | 0.62          |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2  | 2        | 0.62          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2  | 18       | 0.62          |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2  | 11       | 0.62          |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2  | 18       | 0.62          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2  | 1        | 0.62          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2  | 4        | 0.62          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2  | 8        | 0.62          |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3  | 10       | 0.62          |
| (1,288)  | 1:16:A:PHE:HA  | 1:64:A:LEU:HD23 | 12       | 0.62          |
| (1,286)  | 1:16:A:PHE:HA  | 1:64:A:LEU:HD22 | 10       | 0.62          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 6        | 0.62          |
| (1,277)  | 1:111:A:THR:H  | 1:110:A:PRO:HB3 | 18       | 0.62          |
| (1,83)   | 1:46:A:TYR:HD1 | 1:76:A:PRO:HD3  | 8        | 0.62          |
| (1,83)   | 1:46:A:TYR:HD2 | 1:76:A:PRO:HD3  | 8        | 0.62          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 2        | 0.61          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 4        | 0.61          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 6        | 0.61          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 9        | 0.61          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 13       | 0.61          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 16       | 0.61          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 17       | 0.61          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB   | 19       | 0.61          |
| (2,1043) | 1:52:A:SER:H   | 1:63:A:LEU:CB   | 5        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 3        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 3        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 7        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 7        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 8        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 8        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 9        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 9        | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 11       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 11       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 12       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 12       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 14       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 14       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 15       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 15       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 16       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 16       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 18       | 0.61          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA    | 18       | 0.61          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,897)  | 1:64:A:LEU:CB   | 1:65:A:PRO:CB   | 16       | 0.61          |
| (2,853)  | 1:6:A:HIS:CB    | 1:4:A:ILE:CB    | 10       | 0.61          |
| (2,788)  | 1:92:A:VAL:H    | 1:90:A:PHE:CB   | 12       | 0.61          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 15       | 0.61          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 11       | 0.61          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 16       | 0.61          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB   | 1        | 0.61          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB  | 5        | 0.61          |
| (2,627)  | 1:52:A:SER:H    | 1:63:A:LEU:CB   | 5        | 0.61          |
| (2,584)  | 1:108:A:ARG:CB  | 1:9:A:TRP:CB    | 3        | 0.61          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 13       | 0.61          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 11       | 0.61          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 4        | 0.61          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 5        | 0.61          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 10       | 0.61          |
| (2,221)  | 1:30:A:VAL:CA   | 1:31:A:PRO:CB   | 5        | 0.61          |
| (2,188)  | 1:125:A:ILE:CB  | 1:23:A:LYS:CB   | 14       | 0.61          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB   | 6        | 0.61          |
| (2,173)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 1        | 0.61          |
| (2,173)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 4        | 0.61          |
| (2,173)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 5        | 0.61          |
| (2,173)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 11       | 0.61          |
| (2,173)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 16       | 0.61          |
| (2,173)  | 1:110:A:PRO:CB  | 1:109:A:ASP:CA  | 18       | 0.61          |
| (2,84)   | 1:44:A:TYR:CB   | 1:91:A:TRP:CB   | 3        | 0.61          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 18       | 0.61          |
| (1,1269) | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 10       | 0.61          |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12 | 18       | 0.61          |
| (1,1216) | 1:100:A:SER:H   | 1:42:A:LYS:HE3  | 18       | 0.61          |
| (1,1163) | 1:113:A:GLN:HG3 | 1:110:A:PRO:HB2 | 7        | 0.61          |
| (1,944)  | 1:70:A:TYR:HB2  | 1:76:A:PRO:HD3  | 17       | 0.61          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2  | 9        | 0.61          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2  | 1        | 0.61          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2  | 12       | 0.61          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2  | 14       | 0.61          |
| (1,372)  | 1:97:A:ALA:H    | 1:94:A:ASN:HB2  | 6        | 0.61          |
| (1,372)  | 1:97:A:ALA:H    | 1:94:A:ASN:HB2  | 14       | 0.61          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2  | 15       | 0.61          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 11       | 0.61          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2  | 3        | 0.61          |
| (2,1178) | 1:64:A:LEU:CA   | 1:65:A:PRO:CB   | 1        | 0.6           |
| (2,1178) | 1:64:A:LEU:CA   | 1:65:A:PRO:CB   | 3        | 0.6           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 7        | 0.6           |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 8        | 0.6           |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 10       | 0.6           |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 12       | 0.6           |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 14       | 0.6           |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 15       | 0.6           |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 18       | 0.6           |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB | 12       | 0.6           |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB | 17       | 0.6           |
| (2,1086) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB  | 7        | 0.6           |
| (2,978)  | 1:65:A:PRO:CB  | 1:67:A:TRP:CB  | 17       | 0.6           |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA   | 5        | 0.6           |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA   | 5        | 0.6           |
| (2,854)  | 1:14:A:THR:CA  | 1:66:A:ARG:CB  | 12       | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 5        | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 7        | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 8        | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 11       | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 14       | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 15       | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 16       | 0.6           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 18       | 0.6           |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB  | 10       | 0.6           |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB  | 14       | 0.6           |
| (2,783)  | 1:124:A:THR:CB | 1:24:A:PHE:CB  | 10       | 0.6           |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB  | 16       | 0.6           |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB  | 4        | 0.6           |
| (2,594)  | 1:29:A:GLY:H   | 1:92:A:VAL:CB  | 2        | 0.6           |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB  | 17       | 0.6           |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB | 9        | 0.6           |
| (2,338)  | 1:66:A:ARG:H   | 1:48:A:HIS:CB  | 4        | 0.6           |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB  | 8        | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 2        | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 3        | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 6        | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 8        | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 10       | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 13       | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 17       | 0.6           |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA | 19       | 0.6           |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB  | 4        | 0.6           |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB  | 5        | 0.6           |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 8        | 0.6           |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 12       | 0.6           |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 14       | 0.6           |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 16       | 0.6           |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 19       | 0.6           |
| (1,1269) | 1:20:A:ARG:HG2 | 1:128:A:GLN:HG3  | 1        | 0.6           |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12  | 2        | 0.6           |
| (1,1121) | 1:130:A:TYR:H  | 1:127:A:PRO:HG3  | 3        | 0.6           |
| (1,1121) | 1:130:A:TYR:H  | 1:127:A:PRO:HG3  | 8        | 0.6           |
| (1,937)  | 1:69:A:PHE:HB2 | 1:31:A:PRO:HG2   | 9        | 0.6           |
| (1,780)  | 1:131:A:TYR:H  | 1:16:A:PHE:HB3   | 7        | 0.6           |
| (1,776)  | 1:125:A:ILE:H  | 1:25:A:SER:HB3   | 5        | 0.6           |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2   | 6        | 0.6           |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2   | 14       | 0.6           |
| (1,710)  | 1:47:A:ARG:HG2 | 1:67:A:TRP:HE1   | 12       | 0.6           |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2   | 5        | 0.6           |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2   | 19       | 0.6           |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2   | 2        | 0.6           |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2   | 13       | 0.6           |
| (1,192)  | 1:25:A:SER:H   | 1:24:A:PHE:HB3   | 2        | 0.6           |
| (1,47)   | 1:25:A:SER:HA  | 1:28:A:GLN:HB3   | 12       | 0.6           |
| (1,29)   | 1:126:A:LEU:HA | 1:125:A:ILE:HG12 | 4        | 0.6           |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB   | 2        | 0.59          |
| (2,1124) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB    | 18       | 0.59          |
| (2,1124) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB    | 19       | 0.59          |
| (2,1044) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB    | 18       | 0.59          |
| (2,1044) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB    | 19       | 0.59          |
| (2,984)  | 1:119:A:ARG:CB | 1:117:A:PRO:CB   | 8        | 0.59          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA     | 1        | 0.59          |
| (2,954)  | 1:5:A:PRO:CB   | 1:4:A:ILE:CA     | 1        | 0.59          |
| (2,897)  | 1:64:A:LEU:CB  | 1:65:A:PRO:CB    | 1        | 0.59          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 3        | 0.59          |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB     | 12       | 0.59          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB    | 15       | 0.59          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB    | 19       | 0.59          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB    | 7        | 0.59          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB    | 12       | 0.59          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB    | 19       | 0.59          |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB   | 7        | 0.59          |
| (2,727)  | 1:114:A:GLU:CB | 1:116:A:ILE:CB   | 7        | 0.59          |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB    | 6        | 0.59          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB    | 13       | 0.59          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB    | 16       | 0.59          |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB    | 1        | 0.59          |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB    | 11       | 0.59          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 5        | 0.59          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 6        | 0.59          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 14       | 0.59          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB    | 1        | 0.59          |
| (2,366)  | 1:120:A:PHE:CB | 1:31:A:PRO:CB    | 2        | 0.59          |
| (2,366)  | 1:120:A:PHE:CB | 1:31:A:PRO:CB    | 12       | 0.59          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB    | 14       | 0.59          |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB    | 5        | 0.59          |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB    | 11       | 0.59          |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 12       | 0.59          |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 14       | 0.59          |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 15       | 0.59          |
| (2,84)   | 1:44:A:TYR:CB  | 1:91:A:TRP:CB    | 2        | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 2        | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 3        | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 6        | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 7        | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 9        | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 10       | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 13       | 0.59          |
| (2,32)   | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 17       | 0.59          |
| (2,25)   | 1:72:A:LEU:CB  | 1:82:A:TYR:CB    | 19       | 0.59          |
| (2,9)    | 1:4:A:ILE:CB   | 1:6:A:HIS:CB     | 8        | 0.59          |
| (2,9)    | 1:4:A:ILE:CB   | 1:6:A:HIS:CB     | 12       | 0.59          |
| (1,1121) | 1:130:A:TYR:H  | 1:127:A:PRO:HG3  | 11       | 0.59          |
| (1,1121) | 1:130:A:TYR:H  | 1:127:A:PRO:HG3  | 15       | 0.59          |
| (1,941)  | 1:115:A:ALA:HA | 1:114:A:GLU:HG2  | 3        | 0.59          |
| (1,840)  | 1:120:A:PHE:HA | 1:32:A:ILE:HG12  | 4        | 0.59          |
| (1,776)  | 1:125:A:ILE:H  | 1:25:A:SER:HB3   | 4        | 0.59          |
| (1,690)  | 1:99:A:THR:HA  | 1:42:A:LYS:HB3   | 11       | 0.59          |
| (1,517)  | 1:43:A:GLY:HA2 | 1:70:A:TYR:HA    | 9        | 0.59          |
| (1,456)  | 1:132:A:VAL:H  | 1:126:A:LEU:HD22 | 7        | 0.59          |
| (1,388)  | 1:104:A:ASP:H  | 1:40:A:GLU:HB2   | 4        | 0.59          |
| (1,377)  | 1:11:A:SER:H   | 1:10:A:PHE:HB2   | 15       | 0.59          |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2   | 2        | 0.59          |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2   | 9        | 0.59          |
| (1,373)  | 1:96:A:GLN:H   | 1:94:A:ASN:HB2   | 10       | 0.59          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2   | 7        | 0.59          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2   | 10       | 0.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 9        | 0.58          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 6        | 0.58          |
| (2,898)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 2        | 0.58          |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB   | 1        | 0.58          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 12       | 0.58          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 17       | 0.58          |
| (2,838)  | 1:4:A:ILE:CB    | 1:5:A:PRO:CB    | 9        | 0.58          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 16       | 0.58          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 16       | 0.58          |
| (2,775)  | 1:28:A:GLN:H    | 1:25:A:SER:CB   | 2        | 0.58          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB   | 2        | 0.58          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB   | 6        | 0.58          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 4        | 0.58          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB   | 7        | 0.58          |
| (2,676)  | 1:113:A:GLN:CB  | 1:112:A:THR:CB  | 14       | 0.58          |
| (2,676)  | 1:113:A:GLN:CB  | 1:112:A:THR:CB  | 18       | 0.58          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 5        | 0.58          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 6        | 0.58          |
| (2,425)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 8        | 0.58          |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB  | 7        | 0.58          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 13       | 0.58          |
| (2,182)  | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 5        | 0.58          |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 16       | 0.58          |
| (2,32)   | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 1        | 0.58          |
| (2,32)   | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 11       | 0.58          |
| (2,32)   | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 15       | 0.58          |
| (2,32)   | 1:36:A:VAL:CA   | 1:37:A:PRO:CB   | 18       | 0.58          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 14       | 0.58          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 12       | 0.58          |
| (1,1216) | 1:100:A:SER:H   | 1:42:A:LYS:HE3  | 10       | 0.58          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 19       | 0.58          |
| (1,1121) | 1:130:A:TYR:H   | 1:127:A:PRO:HG3 | 9        | 0.58          |
| (1,601)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD23 | 8        | 0.58          |
| (1,377)  | 1:11:A:SER:H    | 1:10:A:PHE:HB2  | 2        | 0.58          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2  | 8        | 0.58          |
| (1,346)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:HA   | 9        | 0.58          |
| (1,281)  | 1:109:A:ASP:H   | 1:108:A:ARG:HB3 | 1        | 0.58          |
| (1,103)  | 1:3:A:THR:HG23  | 1:4:A:ILE:HG23  | 9        | 0.58          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 4        | 0.57          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 15       | 0.57          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 15       | 0.57          |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB  | 11       | 0.57          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 9        | 0.57          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 1        | 0.57          |
| (2,868)  | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 2        | 0.57          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 1        | 0.57          |
| (2,841)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 6        | 0.57          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 11       | 0.57          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 11       | 0.57          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 18       | 0.57          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 18       | 0.57          |
| (2,774)  | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 14       | 0.57          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 2        | 0.57          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB   | 3        | 0.57          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB   | 14       | 0.57          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 3        | 0.57          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 5        | 0.57          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 11       | 0.57          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 14       | 0.57          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB   | 3        | 0.57          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB   | 6        | 0.57          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB   | 9        | 0.57          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB   | 9        | 0.57          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB   | 16       | 0.57          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB   | 17       | 0.57          |
| (2,594)  | 1:29:A:GLY:H    | 1:92:A:VAL:CB   | 18       | 0.57          |
| (2,579)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 9        | 0.57          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 9        | 0.57          |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB  | 16       | 0.57          |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB  | 17       | 0.57          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB   | 17       | 0.57          |
| (2,332)  | 1:4:A:ILE:H     | 1:5:A:PRO:CB    | 9        | 0.57          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 1        | 0.57          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 10       | 0.57          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB   | 15       | 0.57          |
| (2,188)  | 1:125:A:ILE:CB  | 1:23:A:LYS:CB   | 12       | 0.57          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB   | 4        | 0.57          |
| (2,109)  | 1:5:A:PRO:CB    | 1:4:A:ILE:CB    | 2        | 0.57          |
| (2,81)   | 1:9:A:TRP:CB    | 1:71:A:TYR:CB   | 6        | 0.57          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 12       | 0.57          |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12 | 9        | 0.57          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 4        | 0.57          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 13       | 0.57          |
| (1,1128) | 1:73:A:GLY:HA3  | 1:102:A:PRO:HG2 | 9        | 0.57          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1121) | 1:130:A:TYR:H  | 1:127:A:PRO:HG3  | 2        | 0.57          |
| (1,710)  | 1:47:A:ARG:HG2 | 1:67:A:TRP:HE1   | 6        | 0.57          |
| (1,377)  | 1:11:A:SER:H   | 1:10:A:PHE:HB2   | 4        | 0.57          |
| (1,372)  | 1:97:A:ALA:H   | 1:94:A:ASN:HB2   | 17       | 0.57          |
| (1,363)  | 1:66:A:ARG:H   | 1:48:A:HIS:HB3   | 15       | 0.57          |
| (1,334)  | 1:138:A:SER:H  | 1:134:A:GLY:HA3  | 17       | 0.57          |
| (1,42)   | 1:63:A:LEU:HA  | 1:52:A:SER:HB2   | 13       | 0.57          |
| (1,29)   | 1:126:A:LEU:HA | 1:125:A:ILE:HG12 | 16       | 0.57          |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB   | 11       | 0.56          |
| (2,1043) | 1:52:A:SER:H   | 1:63:A:LEU:CB    | 9        | 0.56          |
| (2,856)  | 1:6:A:HIS:CB   | 1:4:A:ILE:CB     | 2        | 0.56          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB   | 8        | 0.56          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB    | 11       | 0.56          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB   | 10       | 0.56          |
| (2,762)  | 1:126:A:LEU:H  | 1:127:A:PRO:CB   | 4        | 0.56          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB    | 8        | 0.56          |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB   | 12       | 0.56          |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB   | 19       | 0.56          |
| (2,689)  | 1:106:A:SER:H  | 1:9:A:TRP:CB     | 11       | 0.56          |
| (2,627)  | 1:52:A:SER:H   | 1:63:A:LEU:CB    | 9        | 0.56          |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB    | 8        | 0.56          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB    | 5        | 0.56          |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB    | 7        | 0.56          |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB    | 14       | 0.56          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 2        | 0.56          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 3        | 0.56          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 8        | 0.56          |
| (2,396)  | 1:15:A:GLN:H   | 1:64:A:LEU:CB    | 8        | 0.56          |
| (2,283)  | 1:81:A:SER:CB  | 1:84:A:GLU:CB    | 15       | 0.56          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB    | 4        | 0.56          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB    | 17       | 0.56          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB    | 19       | 0.56          |
| (2,173)  | 1:110:A:PRO:CB | 1:109:A:ASP:CA   | 9        | 0.56          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB    | 18       | 0.56          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12  | 4        | 0.56          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12  | 7        | 0.56          |
| (1,1238) | 1:120:A:PHE:H  | 1:32:A:ILE:HG12  | 8        | 0.56          |
| (1,1216) | 1:100:A:SER:H  | 1:42:A:LYS:HE3   | 19       | 0.56          |
| (1,941)  | 1:115:A:ALA:HA | 1:114:A:GLU:HG2  | 15       | 0.56          |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2   | 8        | 0.56          |
| (1,720)  | 1:70:A:TYR:H   | 1:31:A:PRO:HG2   | 3        | 0.56          |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2   | 16       | 0.56          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12  | 17       | 0.56          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2   | 16       | 0.56          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2   | 17       | 0.56          |
| (1,372)  | 1:97:A:ALA:H    | 1:94:A:ASN:HB2   | 5        | 0.56          |
| (1,310)  | 1:46:A:TYR:HB2  | 1:68:A:TYR:HB2   | 10       | 0.56          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2   | 2        | 0.56          |
| (1,39)   | 1:32:A:ILE:HG12 | 1:121:A:PRO:HG2  | 6        | 0.56          |
| (1,29)   | 1:126:A:LEU:HA  | 1:125:A:ILE:HG12 | 7        | 0.56          |
| (2,1178) | 1:64:A:LEU:CA   | 1:65:A:PRO:CB    | 11       | 0.55          |
| (2,1125) | 1:127:A:PRO:CB  | 1:126:A:LEU:CB   | 8        | 0.55          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB    | 6        | 0.55          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB    | 6        | 0.55          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 13       | 0.55          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 13       | 0.55          |
| (2,788)  | 1:92:A:VAL:H    | 1:90:A:PHE:CB    | 16       | 0.55          |
| (2,775)  | 1:28:A:GLN:H    | 1:25:A:SER:CB    | 7        | 0.55          |
| (2,774)  | 1:120:A:PHE:CB  | 1:121:A:PRO:CB   | 2        | 0.55          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB    | 2        | 0.55          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB    | 17       | 0.55          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB   | 9        | 0.55          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB   | 10       | 0.55          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB   | 13       | 0.55          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB    | 11       | 0.55          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB    | 4        | 0.55          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB    | 10       | 0.55          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB    | 12       | 0.55          |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB   | 15       | 0.55          |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB   | 18       | 0.55          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB    | 14       | 0.55          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB   | 7        | 0.55          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 19       | 0.55          |
| (2,240)  | 1:20:A:ARG:H    | 1:17:A:GLN:CB    | 19       | 0.55          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB    | 12       | 0.55          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB    | 16       | 0.55          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB    | 18       | 0.55          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB    | 12       | 0.55          |
| (2,164)  | 1:69:A:PHE:CB   | 1:10:A:PHE:CB    | 11       | 0.55          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB    | 5        | 0.55          |
| (2,68)   | 1:86:A:LEU:H    | 1:45:A:TRP:CB    | 16       | 0.55          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB     | 7        | 0.55          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3   | 1        | 0.55          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1   | 9        | 0.55          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 5        | 0.55          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2  | 6        | 0.55          |
| (1,372)  | 1:97:A:ALA:H    | 1:94:A:ASN:HB2  | 11       | 0.55          |
| (1,363)  | 1:66:A:ARG:H    | 1:48:A:HIS:HB3  | 18       | 0.55          |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2  | 3        | 0.55          |
| (1,281)  | 1:109:A:ASP:H   | 1:108:A:ARG:HB3 | 15       | 0.55          |
| (2,1195) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 6        | 0.54          |
| (2,1125) | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 3        | 0.54          |
| (2,1125) | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 5        | 0.54          |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 3        | 0.54          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 6        | 0.54          |
| (2,808)  | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 10       | 0.54          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 9        | 0.54          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 9        | 0.54          |
| (2,788)  | 1:92:A:VAL:H    | 1:90:A:PHE:CB   | 1        | 0.54          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 8        | 0.54          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 14       | 0.54          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 18       | 0.54          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 5        | 0.54          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB   | 15       | 0.54          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 15       | 0.54          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 18       | 0.54          |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB  | 1        | 0.54          |
| (2,676)  | 1:113:A:GLN:CB  | 1:112:A:THR:CB  | 16       | 0.54          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB   | 7        | 0.54          |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 18       | 0.54          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 6        | 0.54          |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 18       | 0.54          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 3        | 0.54          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 8        | 0.54          |
| (2,379)  | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 11       | 0.54          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 9        | 0.54          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB   | 6        | 0.54          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB   | 10       | 0.54          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 16       | 0.54          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 14       | 0.54          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 3        | 0.54          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2   | 10       | 0.54          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2   | 19       | 0.54          |
| (1,955)  | 1:13:A:ILE:HA   | 1:66:A:ARG:HG2  | 8        | 0.54          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2  | 2        | 0.54          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 6        | 0.54          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 8        | 0.54          |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 17       | 0.54          |
| (1,710)  | 1:47:A:ARG:HG2  | 1:67:A:TRP:HE1  | 5        | 0.54          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 19       | 0.54          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2  | 7        | 0.54          |
| (1,372)  | 1:97:A:ALA:H    | 1:94:A:ASN:HB2  | 19       | 0.54          |
| (1,39)   | 1:32:A:ILE:HG12 | 1:121:A:PRO:HG2 | 8        | 0.54          |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2 | 12       | 0.54          |
| (2,1125) | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 4        | 0.53          |
| (2,1125) | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 10       | 0.53          |
| (2,1125) | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 13       | 0.53          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 3        | 0.53          |
| (2,1018) | 1:50:A:ARG:CB   | 1:66:A:ARG:CB   | 6        | 0.53          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 5        | 0.53          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 5        | 0.53          |
| (2,775)  | 1:28:A:GLN:H    | 1:25:A:SER:CB   | 8        | 0.53          |
| (2,774)  | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 15       | 0.53          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 12       | 0.53          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 15       | 0.53          |
| (2,738)  | 1:13:A:ILE:H    | 1:132:A:VAL:CB  | 17       | 0.53          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB   | 14       | 0.53          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 4        | 0.53          |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 11       | 0.53          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 15       | 0.53          |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB  | 19       | 0.53          |
| (2,404)  | 1:71:A:TYR:H    | 1:74:A:THR:CB   | 12       | 0.53          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 6        | 0.53          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 2        | 0.53          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB   | 1        | 0.53          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB   | 8        | 0.53          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 17       | 0.53          |
| (1,1333) | 1:130:A:TYR:HB2 | 1:16:A:PHE:HB3  | 8        | 0.53          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 18       | 0.53          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 17       | 0.53          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2   | 4        | 0.53          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2   | 13       | 0.53          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3  | 9        | 0.53          |
| (1,720)  | 1:70:A:TYR:H    | 1:31:A:PRO:HG2  | 7        | 0.53          |
| (1,601)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD23 | 11       | 0.53          |
| (1,373)  | 1:96:A:GLN:H    | 1:94:A:ASN:HB2  | 13       | 0.53          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2 | 7        | 0.53          |
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB   | 2        | 0.52          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 7        | 0.52          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 9        | 0.52          |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB  | 15       | 0.52          |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB  | 16       | 0.52          |
| (2,1102) | 1:130:A:TYR:H  | 1:17:A:GLN:CB   | 8        | 0.52          |
| (2,1099) | 1:120:A:PHE:H  | 1:32:A:ILE:CB   | 19       | 0.52          |
| (2,841)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 1        | 0.52          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB  | 4        | 0.52          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB  | 4        | 0.52          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB   | 14       | 0.52          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 3        | 0.52          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 11       | 0.52          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB   | 11       | 0.52          |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB   | 8        | 0.52          |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB   | 14       | 0.52          |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB   | 18       | 0.52          |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB   | 3        | 0.52          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 2        | 0.52          |
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB   | 11       | 0.52          |
| (2,443)  | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 1        | 0.52          |
| (2,425)  | 1:132:A:VAL:H  | 1:126:A:LEU:CB  | 16       | 0.52          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB  | 10       | 0.52          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB  | 11       | 0.52          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB   | 6        | 0.52          |
| (2,338)  | 1:66:A:ARG:H   | 1:48:A:HIS:CB   | 2        | 0.52          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB   | 3        | 0.52          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB   | 5        | 0.52          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB   | 9        | 0.52          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB   | 13       | 0.52          |
| (2,164)  | 1:69:A:PHE:CB  | 1:10:A:PHE:CB   | 1        | 0.52          |
| (2,105)  | 1:24:A:PHE:CA  | 1:125:A:ILE:CB  | 8        | 0.52          |
| (2,105)  | 1:24:A:PHE:CA  | 1:125:A:ILE:CB  | 17       | 0.52          |
| (2,102)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB   | 7        | 0.52          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB   | 11       | 0.52          |
| (2,3)    | 1:46:A:TYR:CB  | 1:76:A:PRO:CB   | 17       | 0.52          |
| (1,1334) | 1:16:A:PHE:HB3 | 1:130:A:TYR:HB3 | 2        | 0.52          |
| (1,1242) | 1:130:A:TYR:H  | 1:17:A:GLN:HB2  | 15       | 0.52          |
| (1,1242) | 1:130:A:TYR:H  | 1:17:A:GLN:HB2  | 17       | 0.52          |
| (1,1038) | 1:60:A:GLN:HB3 | 1:54:A:LYS:HE2  | 6        | 0.52          |
| (1,1038) | 1:60:A:GLN:HB3 | 1:54:A:LYS:HE3  | 6        | 0.52          |
| (1,970)  | 1:4:A:ILE:HB   | 1:6:A:HIS:HD2   | 1        | 0.52          |
| (1,970)  | 1:4:A:ILE:HB   | 1:6:A:HIS:HD2   | 17       | 0.52          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,954)  | 1:14:A:THR:HA  | 1:66:A:ARG:HG2  | 8        | 0.52          |
| (1,941)  | 1:115:A:ALA:HA | 1:114:A:GLU:HG2 | 7        | 0.52          |
| (1,888)  | 1:20:A:ARG:HD2 | 1:128:A:GLN:HG3 | 10       | 0.52          |
| (1,876)  | 1:10:A:PHE:H   | 1:8:A:SER:HB3   | 8        | 0.52          |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2  | 13       | 0.52          |
| (1,790)  | 1:42:A:LYS:H   | 1:40:A:GLU:HB2  | 17       | 0.52          |
| (1,377)  | 1:11:A:SER:H   | 1:10:A:PHE:HB2  | 6        | 0.52          |
| (1,377)  | 1:11:A:SER:H   | 1:10:A:PHE:HB2  | 10       | 0.52          |
| (1,288)  | 1:16:A:PHE:HA  | 1:64:A:LEU:HD23 | 19       | 0.52          |
| (1,192)  | 1:25:A:SER:H   | 1:24:A:PHE:HB3  | 11       | 0.52          |
| (1,147)  | 1:4:A:ILE:H    | 1:3:A:THR:HA    | 9        | 0.52          |
| (1,54)   | 1:63:A:LEU:HA  | 1:62:A:GLN:HG2  | 16       | 0.52          |
| (1,26)   | 1:115:A:ALA:H  | 1:114:A:GLU:HG2 | 10       | 0.52          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 18       | 0.51          |
| (2,1138) | 1:103:A:SER:CA | 1:42:A:LYS:CB   | 1        | 0.51          |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB  | 18       | 0.51          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB   | 12       | 0.51          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB   | 15       | 0.51          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 13       | 0.51          |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB   | 3        | 0.51          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB   | 4        | 0.51          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB   | 16       | 0.51          |
| (2,738)  | 1:13:A:ILE:H   | 1:132:A:VAL:CB  | 2        | 0.51          |
| (2,727)  | 1:114:A:GLU:CB | 1:116:A:ILE:CB  | 16       | 0.51          |
| (2,705)  | 1:125:A:ILE:H  | 1:25:A:SER:CB   | 18       | 0.51          |
| (2,676)  | 1:113:A:GLN:CB | 1:112:A:THR:CB  | 3        | 0.51          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 11       | 0.51          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 18       | 0.51          |
| (2,443)  | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 2        | 0.51          |
| (2,443)  | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 5        | 0.51          |
| (2,443)  | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 13       | 0.51          |
| (2,443)  | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 15       | 0.51          |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB   | 10       | 0.51          |
| (2,403)  | 1:105:A:VAL:H  | 1:74:A:THR:CB   | 13       | 0.51          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB   | 3        | 0.51          |
| (2,366)  | 1:120:A:PHE:CB | 1:31:A:PRO:CB   | 13       | 0.51          |
| (2,105)  | 1:24:A:PHE:CA  | 1:125:A:ILE:CB  | 4        | 0.51          |
| (2,84)   | 1:44:A:TYR:CB  | 1:91:A:TRP:CB   | 17       | 0.51          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB   | 10       | 0.51          |
| (1,1266) | 1:51:A:ARG:HB2 | 1:63:A:LEU:HD21 | 10       | 0.51          |
| (1,1216) | 1:100:A:SER:H  | 1:42:A:LYS:HE3  | 13       | 0.51          |
| (1,1173) | 1:51:A:ARG:HB2 | 1:63:A:LEU:HD21 | 10       | 0.51          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1121) | 1:130:A:TYR:H    | 1:127:A:PRO:HG3 | 12       | 0.51          |
| (1,970)  | 1:4:A:ILE:HB     | 1:6:A:HIS:HD2   | 6        | 0.51          |
| (1,941)  | 1:115:A:ALA:HA   | 1:114:A:GLU:HG2 | 8        | 0.51          |
| (1,790)  | 1:42:A:LYS:H     | 1:40:A:GLU:HB2  | 6        | 0.51          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1  | 16       | 0.51          |
| (1,601)  | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD23 | 18       | 0.51          |
| (1,377)  | 1:11:A:SER:H     | 1:10:A:PHE:HB2  | 8        | 0.51          |
| (1,377)  | 1:11:A:SER:H     | 1:10:A:PHE:HB2  | 18       | 0.51          |
| (1,373)  | 1:96:A:GLN:H     | 1:94:A:ASN:HB2  | 4        | 0.51          |
| (1,349)  | 1:63:A:LEU:H     | 1:52:A:SER:HB2  | 14       | 0.51          |
| (1,292)  | 1:17:A:GLN:H     | 1:16:A:PHE:HB3  | 15       | 0.51          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3  | 3        | 0.51          |
| (1,141)  | 1:63:A:LEU:H     | 1:62:A:GLN:HA   | 12       | 0.51          |
| (1,39)   | 1:32:A:ILE:HG12  | 1:121:A:PRO:HG2 | 9        | 0.51          |
| (2,1195) | 1:120:A:PHE:CB   | 1:121:A:PRO:CB  | 8        | 0.5           |
| (2,1124) | 1:51:A:ARG:CB    | 1:63:A:LEU:CB   | 16       | 0.5           |
| (2,1099) | 1:120:A:PHE:H    | 1:32:A:ILE:CB   | 7        | 0.5           |
| (2,1066) | 1:108:A:ARG:CA   | 1:9:A:TRP:CB    | 7        | 0.5           |
| (2,1044) | 1:51:A:ARG:CB    | 1:63:A:LEU:CB   | 16       | 0.5           |
| (2,926)  | 1:101:A:THR:CB   | 1:100:A:SER:CB  | 5        | 0.5           |
| (2,926)  | 1:101:A:THR:CB   | 1:100:A:SER:CB  | 16       | 0.5           |
| (2,897)  | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 10       | 0.5           |
| (2,897)  | 1:64:A:LEU:CB    | 1:65:A:PRO:CB   | 15       | 0.5           |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB  | 16       | 0.5           |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB  | 16       | 0.5           |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB  | 18       | 0.5           |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB  | 18       | 0.5           |
| (2,788)  | 1:92:A:VAL:H     | 1:90:A:PHE:CB   | 4        | 0.5           |
| (2,788)  | 1:92:A:VAL:H     | 1:90:A:PHE:CB   | 9        | 0.5           |
| (2,775)  | 1:28:A:GLN:H     | 1:25:A:SER:CB   | 10       | 0.5           |
| (2,775)  | 1:28:A:GLN:H     | 1:25:A:SER:CB   | 13       | 0.5           |
| (2,774)  | 1:120:A:PHE:CB   | 1:121:A:PRO:CB  | 4        | 0.5           |
| (2,774)  | 1:120:A:PHE:CB   | 1:121:A:PRO:CB  | 5        | 0.5           |
| (2,764)  | 1:120:A:PHE:CA   | 1:32:A:ILE:CB   | 9        | 0.5           |
| (2,762)  | 1:126:A:LEU:H    | 1:127:A:PRO:CB  | 12       | 0.5           |
| (2,745)  | 1:41:A:ALA:H     | 1:30:A:VAL:CB   | 10       | 0.5           |
| (2,721)  | 1:45:A:TRP:H     | 1:89:A:VAL:CB   | 13       | 0.5           |
| (2,621)  | 1:97:A:ALA:CB    | 1:99:A:THR:CB   | 15       | 0.5           |
| (2,560)  | 1:84:A:GLU:H     | 1:91:A:TRP:CB   | 2        | 0.5           |
| (2,526)  | 1:39:A:SER:H     | 1:96:A:GLN:CB   | 19       | 0.5           |
| (2,526)  | 1:39:A:SER:H     | 1:96:A:GLN:CB   | 19       | 0.5           |
| (2,443)  | 1:36:A:VAL:CB    | 1:37:A:PRO:CB   | 3        | 0.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 6        | 0.5           |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 7        | 0.5           |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 9        | 0.5           |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 12       | 0.5           |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 17       | 0.5           |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB  | 13       | 0.5           |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 15       | 0.5           |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 5        | 0.5           |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 16       | 0.5           |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 12       | 0.5           |
| (2,105)  | 1:24:A:PHE:CA   | 1:125:A:ILE:CB  | 18       | 0.5           |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 2        | 0.5           |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB   | 7        | 0.5           |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 3        | 0.5           |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 12       | 0.5           |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 19       | 0.5           |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 17       | 0.5           |
| (1,1269) | 1:20:A:ARG:HG2  | 1:128:A:GLN:HG3 | 15       | 0.5           |
| (1,1238) | 1:120:A:PHE:H   | 1:32:A:ILE:HG12 | 5        | 0.5           |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2  | 13       | 0.5           |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 9        | 0.5           |
| (1,601)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD23 | 3        | 0.5           |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 7        | 0.5           |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2  | 16       | 0.5           |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1  | 10       | 0.5           |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2  | 10       | 0.5           |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 10       | 0.5           |
| (1,363)  | 1:66:A:ARG:H    | 1:48:A:HIS:HB3  | 11       | 0.5           |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB  | 9        | 0.49          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 4        | 0.49          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 2        | 0.49          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 6        | 0.49          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 9        | 0.49          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 14       | 0.49          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 18       | 0.49          |
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 14       | 0.49          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 9        | 0.49          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 12       | 0.49          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 12       | 0.49          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 17       | 0.49          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 17       | 0.49          |
| (2,776)  | 1:28:A:GLN:H    | 1:30:A:VAL:CB   | 12       | 0.49          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,774)  | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 1        | 0.49          |
| (2,774)  | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 16       | 0.49          |
| (2,774)  | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 17       | 0.49          |
| (2,774)  | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 19       | 0.49          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 5        | 0.49          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB   | 9        | 0.49          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB   | 19       | 0.49          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB   | 17       | 0.49          |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 10       | 0.49          |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 14       | 0.49          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB   | 2        | 0.49          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 16       | 0.49          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 2        | 0.49          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 6        | 0.49          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 9        | 0.49          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 14       | 0.49          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 18       | 0.49          |
| (2,237)  | 1:24:A:PHE:H    | 1:90:A:PHE:CB   | 19       | 0.49          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB   | 13       | 0.49          |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 1        | 0.49          |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 7        | 0.49          |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 16       | 0.49          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 9        | 0.49          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 4        | 0.49          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 14       | 0.49          |
| (1,1216) | 1:100:A:SER:H   | 1:42:A:LYS:HE3  | 11       | 0.49          |
| (1,1140) | 1:50:A:ARG:HB3  | 1:66:A:ARG:HD2  | 9        | 0.49          |
| (1,1140) | 1:50:A:ARG:HB2  | 1:66:A:ARG:HD2  | 9        | 0.49          |
| (1,1121) | 1:130:A:TYR:H   | 1:127:A:PRO:HG3 | 1        | 0.49          |
| (1,941)  | 1:115:A:ALA:HA  | 1:114:A:GLU:HG2 | 10       | 0.49          |
| (1,941)  | 1:115:A:ALA:HA  | 1:114:A:GLU:HG2 | 14       | 0.49          |
| (1,851)  | 1:28:A:GLN:H    | 1:25:A:SER:HB3  | 19       | 0.49          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2  | 14       | 0.49          |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 1        | 0.49          |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 18       | 0.49          |
| (1,690)  | 1:99:A:THR:HA   | 1:42:A:LYS:HB3  | 19       | 0.49          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 16       | 0.49          |
| (1,377)  | 1:11:A:SER:H    | 1:10:A:PHE:HB2  | 5        | 0.49          |
| (1,377)  | 1:11:A:SER:H    | 1:10:A:PHE:HB2  | 13       | 0.49          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3  | 19       | 0.49          |
| (2,1125) | 1:127:A:PRO:CB  | 1:126:A:LEU:CB  | 6        | 0.48          |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 17       | 0.48          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,1059) | 1:48:A:HIS:H   | 1:46:A:TYR:CB  | 10       | 0.48          |
| (2,984)  | 1:119:A:ARG:CB | 1:117:A:PRO:CB | 5        | 0.48          |
| (2,984)  | 1:119:A:ARG:CB | 1:117:A:PRO:CB | 16       | 0.48          |
| (2,926)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 7        | 0.48          |
| (2,926)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 15       | 0.48          |
| (2,926)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 17       | 0.48          |
| (2,891)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB  | 4        | 0.48          |
| (2,886)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB  | 14       | 0.48          |
| (2,868)  | 1:4:A:ILE:CB   | 1:6:A:HIS:CB   | 1        | 0.48          |
| (2,860)  | 1:130:A:TYR:CB | 1:20:A:ARG:CB  | 14       | 0.48          |
| (2,856)  | 1:6:A:HIS:CB   | 1:4:A:ILE:CB   | 1        | 0.48          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 2        | 0.48          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 2        | 0.48          |
| (2,783)  | 1:124:A:THR:CB | 1:24:A:PHE:CB  | 6        | 0.48          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB  | 4        | 0.48          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB  | 17       | 0.48          |
| (2,774)  | 1:120:A:PHE:CB | 1:121:A:PRO:CB | 12       | 0.48          |
| (2,584)  | 1:108:A:ARG:CB | 1:9:A:TRP:CB   | 13       | 0.48          |
| (2,583)  | 1:105:A:VAL:CB | 1:9:A:TRP:CB   | 4        | 0.48          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB  | 12       | 0.48          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB  | 17       | 0.48          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB  | 18       | 0.48          |
| (2,241)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 7        | 0.48          |
| (2,241)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 15       | 0.48          |
| (2,241)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 17       | 0.48          |
| (2,205)  | 1:43:A:GLY:H   | 1:92:A:VAL:CB  | 7        | 0.48          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB  | 14       | 0.48          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB  | 15       | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 2        | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 4        | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 5        | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 8        | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 10       | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 11       | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 13       | 0.48          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 15       | 0.48          |
| (2,9)    | 1:4:A:ILE:CB   | 1:6:A:HIS:CB   | 11       | 0.48          |
| (2,3)    | 1:46:A:TYR:CB  | 1:76:A:PRO:CB  | 15       | 0.48          |
| (1,1140) | 1:50:A:ARG:HB3 | 1:66:A:ARG:HD2 | 12       | 0.48          |
| (1,1140) | 1:50:A:ARG:HB2 | 1:66:A:ARG:HD2 | 12       | 0.48          |
| (1,1138) | 1:63:A:LEU:H   | 1:62:A:GLN:HA  | 12       | 0.48          |
| (1,716)  | 1:68:A:TYR:H   | 1:46:A:TYR:HB2 | 3        | 0.48          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 8        | 0.48          |
| (1,601)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD23 | 9        | 0.48          |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23 | 15       | 0.48          |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23 | 19       | 0.48          |
| (1,469)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD22 | 12       | 0.48          |
| (1,377)  | 1:11:A:SER:H    | 1:10:A:PHE:HB2  | 16       | 0.48          |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2  | 8        | 0.48          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3  | 14       | 0.48          |
| (2,930)  | 1:64:A:LEU:CB   | 1:18:A:LYS:CB   | 10       | 0.47          |
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 3        | 0.47          |
| (2,887)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB   | 9        | 0.47          |
| (2,865)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB   | 9        | 0.47          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 13       | 0.47          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 13       | 0.47          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB   | 5        | 0.47          |
| (2,676)  | 1:113:A:GLN:CB  | 1:112:A:THR:CB  | 19       | 0.47          |
| (2,621)  | 1:97:A:ALA:CB   | 1:99:A:THR:CB   | 19       | 0.47          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 3        | 0.47          |
| (2,583)  | 1:105:A:VAL:CB  | 1:9:A:TRP:CB    | 14       | 0.47          |
| (2,404)  | 1:71:A:TYR:H    | 1:74:A:THR:CB   | 8        | 0.47          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 14       | 0.47          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB   | 10       | 0.47          |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 6        | 0.47          |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB   | 9        | 0.47          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 2        | 0.47          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 5        | 0.47          |
| (1,1272) | 1:129:A:GLY:HA3 | 1:17:A:GLN:HB2  | 1        | 0.47          |
| (1,1241) | 1:130:A:TYR:H   | 1:127:A:PRO:HB3 | 5        | 0.47          |
| (1,1199) | 1:9:A:TRP:HE1   | 1:108:A:ARG:HD3 | 15       | 0.47          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 2        | 0.47          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3 | 19       | 0.47          |
| (1,1128) | 1:73:A:GLY:HA3  | 1:102:A:PRO:HG2 | 3        | 0.47          |
| (1,950)  | 1:8:A:SER:HB2   | 1:7:A:TYR:HA    | 8        | 0.47          |
| (1,856)  | 1:81:A:SER:HB2  | 1:82:A:TYR:HA   | 19       | 0.47          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2  | 15       | 0.47          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 6        | 0.47          |
| (1,776)  | 1:125:A:ILE:H   | 1:25:A:SER:HB3  | 3        | 0.47          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 6        | 0.47          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 16       | 0.47          |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 15       | 0.47          |
| (1,654)  | 1:16:A:PHE:H    | 1:64:A:LEU:HD23 | 10       | 0.47          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 10       | 0.47          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,469)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD22  | 14       | 0.47          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2   | 2        | 0.47          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2   | 19       | 0.47          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12  | 6        | 0.47          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3   | 19       | 0.47          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 5        | 0.47          |
| (1,39)   | 1:32:A:ILE:HG12 | 1:121:A:PRO:HG2  | 18       | 0.47          |
| (1,33)   | 1:16:A:PHE:H    | 1:17:A:GLN:HB2   | 3        | 0.47          |
| (2,1126) | 1:20:A:ARG:CB   | 1:128:A:GLN:CB   | 4        | 0.46          |
| (2,887)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB    | 3        | 0.46          |
| (2,865)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB    | 3        | 0.46          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 9        | 0.46          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 9        | 0.46          |
| (2,775)  | 1:28:A:GLN:H    | 1:25:A:SER:CB    | 5        | 0.46          |
| (2,727)  | 1:114:A:GLU:CB  | 1:116:A:ILE:CB   | 15       | 0.46          |
| (2,721)  | 1:45:A:TRP:H    | 1:89:A:VAL:CB    | 1        | 0.46          |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB    | 8        | 0.46          |
| (2,416)  | 1:100:A:SER:H   | 1:101:A:THR:CB   | 4        | 0.46          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB    | 10       | 0.46          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 11       | 0.46          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB    | 5        | 0.46          |
| (2,346)  | 1:97:A:ALA:H    | 1:94:A:ASN:CB    | 3        | 0.46          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB    | 2        | 0.46          |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB    | 1        | 0.46          |
| (2,20)   | 1:30:A:VAL:CB   | 1:31:A:PRO:CB    | 14       | 0.46          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB     | 3        | 0.46          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3   | 3        | 0.46          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3   | 5        | 0.46          |
| (1,924)  | 1:71:A:TYR:HD2  | 1:105:A:VAL:HG23 | 4        | 0.46          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2   | 5        | 0.46          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2   | 12       | 0.46          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2   | 16       | 0.46          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3   | 13       | 0.46          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA    | 14       | 0.46          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA    | 17       | 0.46          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2   | 7        | 0.46          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2   | 17       | 0.46          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12  | 9        | 0.46          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3   | 18       | 0.46          |
| (1,288)  | 1:16:A:PHE:HA   | 1:64:A:LEU:HD23  | 2        | 0.46          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 16       | 0.46          |
| (1,104)  | 1:108:A:ARG:H   | 1:106:A:SER:HA   | 17       | 0.46          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,42)   | 1:63:A:LEU:HA  | 1:52:A:SER:HB2 | 2        | 0.46          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB | 10       | 0.45          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB | 14       | 0.45          |
| (2,978)  | 1:65:A:PRO:CB  | 1:67:A:TRP:CB  | 9        | 0.45          |
| (2,956)  | 1:9:A:TRP:CB   | 1:107:A:SER:CB | 11       | 0.45          |
| (2,850)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB   | 15       | 0.45          |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 5        | 0.45          |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 5        | 0.45          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 3        | 0.45          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 3        | 0.45          |
| (2,792)  | 1:108:A:ARG:H  | 1:9:A:TRP:CB   | 17       | 0.45          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB  | 1        | 0.45          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB  | 9        | 0.45          |
| (2,745)  | 1:41:A:ALA:H   | 1:30:A:VAL:CB  | 5        | 0.45          |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB  | 12       | 0.45          |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB  | 13       | 0.45          |
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB  | 2        | 0.45          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB  | 8        | 0.45          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB  | 9        | 0.45          |
| (2,375)  | 1:119:A:ARG:CB | 1:32:A:ILE:CB  | 19       | 0.45          |
| (2,226)  | 1:113:A:GLN:CB | 1:9:A:TRP:CA   | 12       | 0.45          |
| (2,179)  | 1:103:A:SER:H  | 1:72:A:LEU:CB  | 1        | 0.45          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB  | 9        | 0.45          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 17       | 0.45          |
| (2,20)   | 1:30:A:VAL:CB  | 1:31:A:PRO:CB  | 18       | 0.45          |
| (1,1151) | 1:63:A:LEU:HA  | 1:64:A:LEU:H   | 11       | 0.45          |
| (1,955)  | 1:13:A:ILE:HA  | 1:66:A:ARG:HG2 | 6        | 0.45          |
| (1,937)  | 1:69:A:PHE:HB2 | 1:31:A:PRO:HG2 | 18       | 0.45          |
| (1,517)  | 1:43:A:GLY:HA2 | 1:70:A:TYR:HA  | 18       | 0.45          |
| (1,333)  | 1:81:A:SER:HA  | 1:84:A:GLU:HB3 | 2        | 0.45          |
| (1,333)  | 1:81:A:SER:HA  | 1:84:A:GLU:HB3 | 17       | 0.45          |
| (1,192)  | 1:25:A:SER:H   | 1:24:A:PHE:HB3 | 9        | 0.45          |
| (1,192)  | 1:25:A:SER:H   | 1:24:A:PHE:HB3 | 10       | 0.45          |
| (1,95)   | 1:34:A:PHE:HD2 | 1:71:A:TYR:HE1 | 14       | 0.45          |
| (2,1201) | 1:52:A:SER:CB  | 1:62:A:GLN:CB  | 11       | 0.44          |
| (2,1178) | 1:64:A:LEU:CA  | 1:65:A:PRO:CB  | 5        | 0.44          |
| (2,1126) | 1:20:A:ARG:CB  | 1:128:A:GLN:CB | 5        | 0.44          |
| (2,1099) | 1:120:A:PHE:H  | 1:32:A:ILE:CB  | 18       | 0.44          |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 4        | 0.44          |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 4        | 0.44          |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB  | 13       | 0.44          |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB  | 15       | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,676)  | 1:113:A:GLN:CB  | 1:112:A:THR:CB  | 17       | 0.44          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB   | 7        | 0.44          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB   | 18       | 0.44          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 19       | 0.44          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 4        | 0.44          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB   | 10       | 0.44          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 19       | 0.44          |
| (2,263)  | 1:16:A:PHE:CA   | 1:64:A:LEU:CB   | 8        | 0.44          |
| (2,205)  | 1:43:A:GLY:H    | 1:92:A:VAL:CB   | 11       | 0.44          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB   | 19       | 0.44          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB   | 3        | 0.44          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 6        | 0.44          |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 12       | 0.44          |
| (1,1241) | 1:130:A:TYR:H   | 1:127:A:PRO:HB3 | 18       | 0.44          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 6        | 0.44          |
| (1,1161) | 1:62:A:GLN:HG2  | 1:63:A:LEU:HB3  | 8        | 0.44          |
| (1,1146) | 1:52:A:SER:HB2  | 1:63:A:LEU:HG   | 10       | 0.44          |
| (1,1104) | 1:52:A:SER:HA   | 1:51:A:ARG:HG2  | 19       | 0.44          |
| (1,1103) | 1:55:A:THR:H    | 1:54:A:LYS:HD3  | 8        | 0.44          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2 | 12       | 0.44          |
| (1,789)  | 1:83:A:GLY:HA2  | 1:84:A:GLU:HG2  | 13       | 0.44          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 13       | 0.44          |
| (1,631)  | 1:89:A:VAL:HG23 | 1:86:A:LEU:HB3  | 12       | 0.44          |
| (1,601)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD23 | 17       | 0.44          |
| (1,469)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD22 | 5        | 0.44          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2  | 14       | 0.44          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12 | 19       | 0.44          |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2  | 6        | 0.44          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3  | 9        | 0.44          |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 6        | 0.44          |
| (2,1203) | 1:64:A:LEU:CB   | 1:15:A:GLN:CB   | 11       | 0.43          |
| (2,1195) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB  | 2        | 0.43          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 19       | 0.43          |
| (2,1087) | 1:137:A:ARG:H   | 1:11:A:SER:CB   | 19       | 0.43          |
| (2,1086) | 1:47:A:ARG:CB   | 1:67:A:TRP:CB   | 8        | 0.43          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 2        | 0.43          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 5        | 0.43          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 18       | 0.43          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 1        | 0.43          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 1        | 0.43          |
| (2,775)  | 1:28:A:GLN:H    | 1:25:A:SER:CB   | 6        | 0.43          |
| (2,764)  | 1:120:A:PHE:CA  | 1:32:A:ILE:CB   | 1        | 0.43          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,718)  | 1:42:A:LYS:H    | 1:40:A:GLU:CB    | 11       | 0.43          |
| (2,705)  | 1:125:A:ILE:H   | 1:25:A:SER:CB    | 11       | 0.43          |
| (2,697)  | 1:119:A:ARG:H   | 1:31:A:PRO:CB    | 11       | 0.43          |
| (2,654)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB   | 4        | 0.43          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB    | 10       | 0.43          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB    | 14       | 0.43          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 13       | 0.43          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB    | 18       | 0.43          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 4        | 0.43          |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB    | 8        | 0.43          |
| (2,179)  | 1:103:A:SER:H   | 1:72:A:LEU:CB    | 13       | 0.43          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H    | 8        | 0.43          |
| (1,1241) | 1:130:A:TYR:H   | 1:127:A:PRO:HB3  | 6        | 0.43          |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 12       | 0.43          |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 12       | 0.43          |
| (1,856)  | 1:81:A:SER:HB2  | 1:82:A:TYR:HA    | 5        | 0.43          |
| (1,805)  | 1:117:A:PRO:HA  | 1:11:A:SER:HA    | 12       | 0.43          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3   | 8        | 0.43          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3   | 12       | 0.43          |
| (1,631)  | 1:89:A:VAL:HG23 | 1:86:A:LEU:HB3   | 14       | 0.43          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA    | 3        | 0.43          |
| (1,456)  | 1:132:A:VAL:H   | 1:126:A:LEU:HD22 | 1        | 0.43          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2   | 8        | 0.43          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2   | 15       | 0.43          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3   | 3        | 0.43          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3   | 4        | 0.43          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 14       | 0.43          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 15       | 0.43          |
| (1,78)   | 1:82:A:TYR:HB2  | 1:83:A:GLY:HA2   | 8        | 0.43          |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2  | 4        | 0.43          |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2  | 9        | 0.43          |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2  | 14       | 0.43          |
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB    | 3        | 0.42          |
| (2,1195) | 1:120:A:PHE:CB  | 1:121:A:PRO:CB   | 15       | 0.42          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB    | 1        | 0.42          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 8        | 0.42          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 12       | 0.42          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 12       | 0.42          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 12       | 0.42          |
| (2,788)  | 1:92:A:VAL:H    | 1:90:A:PHE:CB    | 13       | 0.42          |
| (2,788)  | 1:92:A:VAL:H    | 1:90:A:PHE:CB    | 17       | 0.42          |
| (2,775)  | 1:28:A:GLN:H    | 1:25:A:SER:CB    | 16       | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,749)  | 1:118:A:THR:CB  | 1:132:A:VAL:CB  | 10       | 0.42          |
| (2,705)  | 1:125:A:ILE:H   | 1:25:A:SER:CB   | 12       | 0.42          |
| (2,685)  | 1:103:A:SER:H   | 1:105:A:VAL:CB  | 5        | 0.42          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB   | 2        | 0.42          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 6        | 0.42          |
| (2,582)  | 1:107:A:SER:CA  | 1:9:A:TRP:CB    | 11       | 0.42          |
| (2,444)  | 1:104:A:ASP:CB  | 1:36:A:VAL:CB   | 3        | 0.42          |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 3        | 0.42          |
| (1,1277) | 1:15:A:GLN:HA   | 1:64:A:LEU:HB3  | 5        | 0.42          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2  | 1        | 0.42          |
| (1,856)  | 1:81:A:SER:HB2  | 1:82:A:TYR:HA   | 12       | 0.42          |
| (1,856)  | 1:81:A:SER:HB2  | 1:82:A:TYR:HA   | 14       | 0.42          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2  | 7        | 0.42          |
| (1,716)  | 1:68:A:TYR:H    | 1:46:A:TYR:HB2  | 7        | 0.42          |
| (1,641)  | 1:108:A:ARG:HB3 | 1:9:A:TRP:HE1   | 3        | 0.42          |
| (1,601)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD23 | 1        | 0.42          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 5        | 0.42          |
| (1,414)  | 1:65:A:PRO:HB3  | 1:67:A:TRP:HE1  | 15       | 0.42          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2  | 1        | 0.42          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2  | 13       | 0.42          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1  | 9        | 0.42          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2  | 9        | 0.42          |
| (1,372)  | 1:97:A:ALA:H    | 1:94:A:ASN:HB2  | 12       | 0.42          |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2  | 7        | 0.42          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3  | 7        | 0.42          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3  | 8        | 0.42          |
| (1,95)   | 1:34:A:PHE:HD2  | 1:71:A:TYR:HE1  | 5        | 0.42          |
| (1,81)   | 1:13:A:ILE:HA   | 1:133:A:GLU:H   | 8        | 0.42          |
| (1,78)   | 1:82:A:TYR:HB2  | 1:83:A:GLY:HA2  | 2        | 0.42          |
| (1,78)   | 1:82:A:TYR:HB2  | 1:83:A:GLY:HA2  | 11       | 0.42          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2  | 18       | 0.42          |
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB   | 8        | 0.41          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB  | 13       | 0.41          |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB   | 18       | 0.41          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 4        | 0.41          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 8        | 0.41          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 10       | 0.41          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 17       | 0.41          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB  | 14       | 0.41          |
| (2,886)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 19       | 0.41          |
| (2,860)  | 1:130:A:TYR:CB  | 1:20:A:ARG:CB   | 19       | 0.41          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB    | 7        | 0.41          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 14       | 0.41          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 17       | 0.41          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 17       | 0.41          |
| (2,788)  | 1:92:A:VAL:H    | 1:90:A:PHE:CB    | 3        | 0.41          |
| (2,745)  | 1:41:A:ALA:H    | 1:30:A:VAL:CB    | 18       | 0.41          |
| (2,718)  | 1:42:A:LYS:H    | 1:40:A:GLU:CB    | 18       | 0.41          |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB    | 16       | 0.41          |
| (2,587)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB    | 16       | 0.41          |
| (2,444)  | 1:104:A:ASP:CB  | 1:36:A:VAL:CB    | 8        | 0.41          |
| (2,428)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB   | 7        | 0.41          |
| (2,375)  | 1:119:A:ARG:CB  | 1:32:A:ILE:CB    | 7        | 0.41          |
| (2,366)  | 1:120:A:PHE:CB  | 1:31:A:PRO:CB    | 3        | 0.41          |
| (2,338)  | 1:66:A:ARG:H    | 1:48:A:HIS:CB    | 11       | 0.41          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB    | 1        | 0.41          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB    | 12       | 0.41          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB    | 19       | 0.41          |
| (1,1103) | 1:55:A:THR:H    | 1:54:A:LYS:HD3   | 15       | 0.41          |
| (1,971)  | 1:63:A:LEU:HA   | 1:64:A:LEU:H     | 11       | 0.41          |
| (1,780)  | 1:131:A:TYR:H   | 1:16:A:PHE:HB3   | 16       | 0.41          |
| (1,705)  | 1:73:A:GLY:HA3  | 1:102:A:PRO:HB2  | 11       | 0.41          |
| (1,533)  | 1:10:A:PHE:HB3  | 1:11:A:SER:HA    | 19       | 0.41          |
| (1,477)  | 1:37:A:PRO:HD3  | 1:36:A:VAL:HG22  | 4        | 0.41          |
| (1,477)  | 1:37:A:PRO:HD3  | 1:36:A:VAL:HG21  | 4        | 0.41          |
| (1,456)  | 1:132:A:VAL:H   | 1:126:A:LEU:HD22 | 19       | 0.41          |
| (1,414)  | 1:65:A:PRO:HB3  | 1:67:A:TRP:HE1   | 10       | 0.41          |
| (1,388)  | 1:104:A:ASP:H   | 1:40:A:GLU:HB2   | 12       | 0.41          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12  | 8        | 0.41          |
| (1,377)  | 1:11:A:SER:H    | 1:10:A:PHE:HB2   | 9        | 0.41          |
| (1,363)  | 1:66:A:ARG:H    | 1:48:A:HIS:HB3   | 10       | 0.41          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2   | 5        | 0.41          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3   | 5        | 0.41          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3   | 11       | 0.41          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3   | 15       | 0.41          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3   | 19       | 0.41          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3   | 14       | 0.41          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3   | 17       | 0.41          |
| (1,288)  | 1:16:A:PHE:HA   | 1:64:A:LEU:HD23  | 17       | 0.41          |
| (1,270)  | 1:112:A:THR:H   | 1:109:A:ASP:HB2  | 6        | 0.41          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 4        | 0.41          |
| (1,39)   | 1:32:A:ILE:HG12 | 1:121:A:PRO:HG2  | 7        | 0.41          |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2  | 1        | 0.41          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB   | 16       | 0.4           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB | 3        | 0.4           |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB | 11       | 0.4           |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB | 9        | 0.4           |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB | 14       | 0.4           |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB | 19       | 0.4           |
| (2,1099) | 1:120:A:PHE:H  | 1:32:A:ILE:CB  | 16       | 0.4           |
| (2,1059) | 1:48:A:HIS:H   | 1:46:A:TYR:CB  | 11       | 0.4           |
| (2,1018) | 1:50:A:ARG:CB  | 1:66:A:ARG:CB  | 2        | 0.4           |
| (2,984)  | 1:119:A:ARG:CB | 1:117:A:PRO:CB | 2        | 0.4           |
| (2,926)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 4        | 0.4           |
| (2,868)  | 1:4:A:ILE:CB   | 1:6:A:HIS:CB   | 10       | 0.4           |
| (2,856)  | 1:6:A:HIS:CB   | 1:4:A:ILE:CB   | 10       | 0.4           |
| (2,850)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB   | 11       | 0.4           |
| (2,838)  | 1:4:A:ILE:CB   | 1:5:A:PRO:CB   | 2        | 0.4           |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 2        | 0.4           |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 2        | 0.4           |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 14       | 0.4           |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB | 14       | 0.4           |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB  | 10       | 0.4           |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB  | 5        | 0.4           |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB  | 15       | 0.4           |
| (2,583)  | 1:105:A:VAL:CB | 1:9:A:TRP:CB   | 16       | 0.4           |
| (2,571)  | 1:89:A:VAL:CB  | 1:45:A:TRP:CB  | 16       | 0.4           |
| (2,564)  | 1:127:A:PRO:CB | 1:23:A:LYS:CB  | 9        | 0.4           |
| (2,440)  | 1:91:A:TRP:H   | 1:89:A:VAL:CB  | 5        | 0.4           |
| (2,425)  | 1:132:A:VAL:H  | 1:126:A:LEU:CB | 18       | 0.4           |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB  | 4        | 0.4           |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB  | 8        | 0.4           |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB  | 16       | 0.4           |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB  | 19       | 0.4           |
| (2,338)  | 1:66:A:ARG:H   | 1:48:A:HIS:CB  | 15       | 0.4           |
| (2,241)  | 1:101:A:THR:CB | 1:100:A:SER:CB | 4        | 0.4           |
| (2,156)  | 1:4:A:ILE:CB   | 1:6:A:HIS:CB   | 9        | 0.4           |
| (2,102)  | 1:48:A:HIS:CB  | 1:68:A:TYR:CB  | 9        | 0.4           |
| (1,1211) | 1:43:A:GLY:H   | 1:72:A:LEU:HB3 | 4        | 0.4           |
| (1,1103) | 1:55:A:THR:H   | 1:54:A:LYS:HD3 | 14       | 0.4           |
| (1,970)  | 1:4:A:ILE:HB   | 1:6:A:HIS:HD2  | 9        | 0.4           |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA  | 2        | 0.4           |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA  | 4        | 0.4           |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA  | 7        | 0.4           |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA  | 9        | 0.4           |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA  | 11       | 0.4           |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA    | 18       | 0.4           |
| (1,780)  | 1:131:A:TYR:H  | 1:16:A:PHE:HB3   | 3        | 0.4           |
| (1,680)  | 1:41:A:ALA:H   | 1:36:A:VAL:HG23  | 5        | 0.4           |
| (1,477)  | 1:37:A:PRO:HD3 | 1:36:A:VAL:HG22  | 16       | 0.4           |
| (1,477)  | 1:37:A:PRO:HD3 | 1:36:A:VAL:HG21  | 16       | 0.4           |
| (1,388)  | 1:104:A:ASP:H  | 1:40:A:GLU:HB2   | 6        | 0.4           |
| (1,380)  | 1:31:A:PRO:HA  | 1:32:A:ILE:HG12  | 18       | 0.4           |
| (1,377)  | 1:11:A:SER:H   | 1:10:A:PHE:HB2   | 7        | 0.4           |
| (1,343)  | 1:97:A:ALA:H   | 1:39:A:SER:HA    | 17       | 0.4           |
| (1,334)  | 1:138:A:SER:H  | 1:134:A:GLY:HA3  | 6        | 0.4           |
| (1,333)  | 1:81:A:SER:HA  | 1:84:A:GLU:HB3   | 12       | 0.4           |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3   | 7        | 0.4           |
| (1,221)  | 1:111:A:THR:H  | 1:110:A:PRO:HG3  | 7        | 0.4           |
| (1,78)   | 1:82:A:TYR:HB2 | 1:83:A:GLY:HA2   | 7        | 0.4           |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB   | 4        | 0.39          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB   | 13       | 0.39          |
| (2,1130) | 1:129:A:GLY:CA | 1:20:A:ARG:CB    | 10       | 0.39          |
| (2,984)  | 1:119:A:ARG:CB | 1:117:A:PRO:CB   | 13       | 0.39          |
| (2,850)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB     | 3        | 0.39          |
| (2,850)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB     | 16       | 0.39          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB    | 11       | 0.39          |
| (2,764)  | 1:120:A:PHE:CA | 1:32:A:ILE:CB    | 11       | 0.39          |
| (2,595)  | 1:17:A:GLN:H   | 1:64:A:LEU:CB    | 17       | 0.39          |
| (2,594)  | 1:29:A:GLY:H   | 1:92:A:VAL:CB    | 8        | 0.39          |
| (2,497)  | 1:54:A:LYS:CB  | 1:60:A:GLN:CB    | 18       | 0.39          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 5        | 0.39          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 6        | 0.39          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 10       | 0.39          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 12       | 0.39          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB    | 14       | 0.39          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 12       | 0.39          |
| (2,188)  | 1:125:A:ILE:CB | 1:23:A:LYS:CB    | 11       | 0.39          |
| (2,105)  | 1:24:A:PHE:CA  | 1:125:A:ILE:CB   | 5        | 0.39          |
| (1,1242) | 1:130:A:TYR:H  | 1:17:A:GLN:HB2   | 13       | 0.39          |
| (1,1103) | 1:55:A:THR:H   | 1:54:A:LYS:HD3   | 16       | 0.39          |
| (1,1016) | 1:126:A:LEU:H  | 1:125:A:ILE:HG12 | 7        | 0.39          |
| (1,924)  | 1:71:A:TYR:HD2 | 1:105:A:VAL:HG23 | 5        | 0.39          |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA    | 1        | 0.39          |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA    | 8        | 0.39          |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA    | 10       | 0.39          |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA    | 15       | 0.39          |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA    | 17       | 0.39          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,840)  | 1:120:A:PHE:HA | 1:32:A:ILE:HG12 | 6        | 0.39          |
| (1,720)  | 1:70:A:TYR:H   | 1:31:A:PRO:HG2  | 13       | 0.39          |
| (1,711)  | 1:47:A:ARG:HA  | 1:67:A:TRP:HE1  | 8        | 0.39          |
| (1,471)  | 1:84:A:GLU:H   | 1:86:A:LEU:HD23 | 4        | 0.39          |
| (1,388)  | 1:104:A:ASP:H  | 1:40:A:GLU:HB2  | 10       | 0.39          |
| (1,388)  | 1:104:A:ASP:H  | 1:40:A:GLU:HB2  | 18       | 0.39          |
| (1,377)  | 1:11:A:SER:H   | 1:10:A:PHE:HB2  | 14       | 0.39          |
| (1,359)  | 1:72:A:LEU:H   | 1:71:A:TYR:HB2  | 14       | 0.39          |
| (1,333)  | 1:81:A:SER:HA  | 1:84:A:GLU:HB3  | 10       | 0.39          |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3  | 1        | 0.39          |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3  | 5        | 0.39          |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3  | 18       | 0.39          |
| (1,288)  | 1:16:A:PHE:HA  | 1:64:A:LEU:HD23 | 18       | 0.39          |
| (1,192)  | 1:25:A:SER:H   | 1:24:A:PHE:HB3  | 17       | 0.39          |
| (1,173)  | 1:36:A:VAL:H   | 1:35:A:GLY:HA2  | 18       | 0.39          |
| (1,54)   | 1:63:A:LEU:HA  | 1:62:A:GLN:HG2  | 15       | 0.39          |
| (1,26)   | 1:115:A:ALA:H  | 1:114:A:GLU:HG2 | 3        | 0.39          |
| (1,26)   | 1:115:A:ALA:H  | 1:114:A:GLU:HG2 | 6        | 0.39          |
| (1,26)   | 1:115:A:ALA:H  | 1:114:A:GLU:HG2 | 7        | 0.39          |
| (1,26)   | 1:115:A:ALA:H  | 1:114:A:GLU:HG2 | 11       | 0.39          |
| (2,1200) | 1:130:A:TYR:CB | 1:126:A:LEU:CB  | 17       | 0.38          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 1        | 0.38          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 5        | 0.38          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 19       | 0.38          |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB  | 7        | 0.38          |
| (2,984)  | 1:119:A:ARG:CB | 1:117:A:PRO:CB  | 18       | 0.38          |
| (2,749)  | 1:118:A:THR:CB | 1:132:A:VAL:CB  | 12       | 0.38          |
| (2,721)  | 1:45:A:TRP:H   | 1:89:A:VAL:CB   | 17       | 0.38          |
| (2,621)  | 1:97:A:ALA:CB  | 1:99:A:THR:CB   | 12       | 0.38          |
| (2,526)  | 1:39:A:SER:H   | 1:96:A:GLN:CB   | 3        | 0.38          |
| (2,526)  | 1:39:A:SER:H   | 1:96:A:GLN:CB   | 3        | 0.38          |
| (2,425)  | 1:132:A:VAL:H  | 1:126:A:LEU:CB  | 6        | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 1        | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 2        | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 3        | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 7        | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 9        | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 11       | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 13       | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 15       | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 17       | 0.38          |
| (2,424)  | 1:36:A:VAL:CA  | 1:37:A:PRO:CB   | 18       | 0.38          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,396)  | 1:15:A:GLN:H   | 1:64:A:LEU:CB    | 16       | 0.38          |
| (2,369)  | 1:96:A:GLN:CB  | 1:38:A:PRO:CB    | 12       | 0.38          |
| (2,366)  | 1:120:A:PHE:CB | 1:31:A:PRO:CB    | 11       | 0.38          |
| (2,263)  | 1:16:A:PHE:CA  | 1:64:A:LEU:CB    | 3        | 0.38          |
| (2,3)    | 1:46:A:TYR:CB  | 1:76:A:PRO:CB    | 7        | 0.38          |
| (1,1334) | 1:16:A:PHE:HB3 | 1:130:A:TYR:HB3  | 7        | 0.38          |
| (1,1103) | 1:55:A:THR:H   | 1:54:A:LYS:HD3   | 2        | 0.38          |
| (1,1016) | 1:126:A:LEU:H  | 1:125:A:ILE:HG12 | 14       | 0.38          |
| (1,1005) | 1:135:A:SER:HA | 1:117:A:PRO:HD2  | 7        | 0.38          |
| (1,856)  | 1:81:A:SER:HB2 | 1:82:A:TYR:HA    | 3        | 0.38          |
| (1,745)  | 1:91:A:TRP:H   | 1:90:A:PHE:HB3   | 2        | 0.38          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23  | 14       | 0.38          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23  | 19       | 0.38          |
| (1,533)  | 1:10:A:PHE:HB3 | 1:11:A:SER:HA    | 1        | 0.38          |
| (1,477)  | 1:37:A:PRO:HD3 | 1:36:A:VAL:HG22  | 19       | 0.38          |
| (1,477)  | 1:37:A:PRO:HD3 | 1:36:A:VAL:HG21  | 19       | 0.38          |
| (1,388)  | 1:104:A:ASP:H  | 1:40:A:GLU:HB2   | 9        | 0.38          |
| (1,343)  | 1:97:A:ALA:H   | 1:39:A:SER:HA    | 7        | 0.38          |
| (1,192)  | 1:25:A:SER:H   | 1:24:A:PHE:HB3   | 13       | 0.38          |
| (1,173)  | 1:36:A:VAL:H   | 1:35:A:GLY:HA2   | 4        | 0.38          |
| (1,173)  | 1:36:A:VAL:H   | 1:35:A:GLY:HA2   | 16       | 0.38          |
| (1,173)  | 1:36:A:VAL:H   | 1:35:A:GLY:HA2   | 19       | 0.38          |
| (1,78)   | 1:82:A:TYR:HB2 | 1:83:A:GLY:HA2   | 17       | 0.38          |
| (1,53)   | 1:138:A:SER:HA | 1:11:A:SER:HB3   | 12       | 0.38          |
| (1,26)   | 1:115:A:ALA:H  | 1:114:A:GLU:HG2  | 8        | 0.38          |
| (2,1201) | 1:52:A:SER:CB  | 1:62:A:GLN:CB    | 9        | 0.37          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB   | 16       | 0.37          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB   | 17       | 0.37          |
| (2,1125) | 1:127:A:PRO:CB | 1:126:A:LEU:CB   | 1        | 0.37          |
| (2,1086) | 1:47:A:ARG:CB  | 1:67:A:TRP:CB    | 9        | 0.37          |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB   | 3        | 0.37          |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB   | 3        | 0.37          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB   | 7        | 0.37          |
| (2,802)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB   | 7        | 0.37          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB    | 8        | 0.37          |
| (2,778)  | 1:29:A:GLY:H   | 1:120:A:PHE:CB   | 9        | 0.37          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB    | 3        | 0.37          |
| (2,718)  | 1:42:A:LYS:H   | 1:40:A:GLU:CB    | 15       | 0.37          |
| (2,583)  | 1:105:A:VAL:CB | 1:9:A:TRP:CB     | 1        | 0.37          |
| (2,537)  | 1:124:A:THR:H  | 1:28:A:GLN:CB    | 4        | 0.37          |
| (2,428)  | 1:132:A:VAL:H  | 1:126:A:LEU:CB   | 1        | 0.37          |
| (2,416)  | 1:100:A:SER:H  | 1:101:A:THR:CB   | 1        | 0.37          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,396)  | 1:15:A:GLN:H   | 1:64:A:LEU:CB   | 9        | 0.37          |
| (2,356)  | 1:31:A:PRO:CB  | 1:120:A:PHE:CB  | 1        | 0.37          |
| (1,1334) | 1:16:A:PHE:HB3 | 1:130:A:TYR:HB3 | 16       | 0.37          |
| (1,1103) | 1:55:A:THR:H   | 1:54:A:LYS:HD3  | 4        | 0.37          |
| (1,805)  | 1:117:A:PRO:HA | 1:11:A:SER:HA   | 13       | 0.37          |
| (1,768)  | 1:119:A:ARG:H  | 1:31:A:PRO:HB3  | 11       | 0.37          |
| (1,422)  | 1:15:A:GLN:H   | 1:64:A:LEU:HB2  | 3        | 0.37          |
| (1,388)  | 1:104:A:ASP:H  | 1:40:A:GLU:HB2  | 3        | 0.37          |
| (1,343)  | 1:97:A:ALA:H   | 1:39:A:SER:HA   | 13       | 0.37          |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3  | 16       | 0.37          |
| (1,281)  | 1:109:A:ASP:H  | 1:108:A:ARG:HB3 | 8        | 0.37          |
| (1,192)  | 1:25:A:SER:H   | 1:24:A:PHE:HB3  | 6        | 0.37          |
| (1,173)  | 1:36:A:VAL:H   | 1:35:A:GLY:HA2  | 3        | 0.37          |
| (1,124)  | 1:5:A:PRO:HD3  | 1:4:A:ILE:HG22  | 17       | 0.37          |
| (1,124)  | 1:5:A:PRO:HD3  | 1:4:A:ILE:HG21  | 17       | 0.37          |
| (1,104)  | 1:108:A:ARG:H  | 1:106:A:SER:HA  | 9        | 0.37          |
| (1,83)   | 1:46:A:TYR:HD1 | 1:76:A:PRO:HD3  | 17       | 0.37          |
| (1,83)   | 1:46:A:TYR:HD2 | 1:76:A:PRO:HD3  | 17       | 0.37          |
| (1,78)   | 1:82:A:TYR:HB2 | 1:83:A:GLY:HA2  | 1        | 0.37          |
| (2,1195) | 1:120:A:PHE:CB | 1:121:A:PRO:CB  | 12       | 0.36          |
| (2,1138) | 1:103:A:SER:CA | 1:42:A:LYS:CB   | 15       | 0.36          |
| (2,1059) | 1:48:A:HIS:H   | 1:46:A:TYR:CB   | 6        | 0.36          |
| (2,853)  | 1:6:A:HIS:CB   | 1:4:A:ILE:CB    | 9        | 0.36          |
| (2,850)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB    | 13       | 0.36          |
| (2,788)  | 1:92:A:VAL:H   | 1:90:A:PHE:CB   | 7        | 0.36          |
| (2,783)  | 1:124:A:THR:CB | 1:24:A:PHE:CB   | 7        | 0.36          |
| (2,718)  | 1:42:A:LYS:H   | 1:40:A:GLU:CB   | 12       | 0.36          |
| (2,583)  | 1:105:A:VAL:CB | 1:9:A:TRP:CB    | 13       | 0.36          |
| (2,425)  | 1:132:A:VAL:H  | 1:126:A:LEU:CB  | 14       | 0.36          |
| (2,362)  | 1:104:A:ASP:H  | 1:40:A:GLU:CB   | 12       | 0.36          |
| (2,324)  | 1:63:A:LEU:H   | 1:52:A:SER:CB   | 14       | 0.36          |
| (2,217)  | 1:89:A:VAL:CB  | 1:45:A:TRP:CB   | 2        | 0.36          |
| (1,1161) | 1:62:A:GLN:HG2 | 1:63:A:LEU:HB3  | 7        | 0.36          |
| (1,1103) | 1:55:A:THR:H   | 1:54:A:LYS:HD3  | 10       | 0.36          |
| (1,1029) | 1:51:A:ARG:HA  | 1:63:A:LEU:HD21 | 15       | 0.36          |
| (1,834)  | 1:118:A:THR:H  | 1:134:A:GLY:HA2 | 16       | 0.36          |
| (1,720)  | 1:70:A:TYR:H   | 1:31:A:PRO:HG2  | 12       | 0.36          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23 | 7        | 0.36          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23 | 10       | 0.36          |
| (1,599)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD22 | 15       | 0.36          |
| (1,359)  | 1:72:A:LEU:H   | 1:71:A:TYR:HB2  | 16       | 0.36          |
| (1,334)  | 1:138:A:SER:H  | 1:134:A:GLY:HA3 | 8        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,333)  | 1:81:A:SER:HA    | 1:84:A:GLU:HB3   | 1        | 0.36          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3   | 2        | 0.36          |
| (1,173)  | 1:36:A:VAL:H     | 1:35:A:GLY:HA2   | 1        | 0.36          |
| (1,173)  | 1:36:A:VAL:H     | 1:35:A:GLY:HA2   | 10       | 0.36          |
| (1,173)  | 1:36:A:VAL:H     | 1:35:A:GLY:HA2   | 17       | 0.36          |
| (1,78)   | 1:82:A:TYR:HB2   | 1:83:A:GLY:HA2   | 5        | 0.36          |
| (1,78)   | 1:82:A:TYR:HB2   | 1:83:A:GLY:HA2   | 10       | 0.36          |
| (1,78)   | 1:82:A:TYR:HB2   | 1:83:A:GLY:HA2   | 18       | 0.36          |
| (1,26)   | 1:115:A:ALA:H    | 1:114:A:GLU:HG2  | 5        | 0.36          |
| (1,26)   | 1:115:A:ALA:H    | 1:114:A:GLU:HG2  | 15       | 0.36          |
| (2,1126) | 1:20:A:ARG:CB    | 1:128:A:GLN:CB   | 13       | 0.35          |
| (2,1102) | 1:130:A:TYR:H    | 1:17:A:GLN:CB    | 12       | 0.35          |
| (2,1099) | 1:120:A:PHE:H    | 1:32:A:ILE:CB    | 9        | 0.35          |
| (2,1066) | 1:108:A:ARG:CA   | 1:9:A:TRP:CB     | 16       | 0.35          |
| (2,987)  | 1:32:A:ILE:CB    | 1:121:A:PRO:CB   | 19       | 0.35          |
| (2,850)  | 1:5:A:PRO:CB     | 1:6:A:HIS:CB     | 6        | 0.35          |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 1        | 0.35          |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 1        | 0.35          |
| (2,802)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 8        | 0.35          |
| (2,802)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 8        | 0.35          |
| (2,802)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 15       | 0.35          |
| (2,802)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 15       | 0.35          |
| (2,749)  | 1:118:A:THR:CB   | 1:132:A:VAL:CB   | 4        | 0.35          |
| (2,685)  | 1:103:A:SER:H    | 1:105:A:VAL:CB   | 4        | 0.35          |
| (2,676)  | 1:113:A:GLN:CB   | 1:112:A:THR:CB   | 2        | 0.35          |
| (2,645)  | 1:68:A:TYR:H     | 1:69:A:PHE:CB    | 6        | 0.35          |
| (2,645)  | 1:68:A:TYR:H     | 1:69:A:PHE:CB    | 16       | 0.35          |
| (2,643)  | 1:68:A:TYR:H     | 1:48:A:HIS:H     | 10       | 0.35          |
| (2,621)  | 1:97:A:ALA:CB    | 1:99:A:THR:CB    | 1        | 0.35          |
| (2,595)  | 1:17:A:GLN:H     | 1:64:A:LEU:CB    | 19       | 0.35          |
| (2,583)  | 1:105:A:VAL:CB   | 1:9:A:TRP:CB     | 11       | 0.35          |
| (2,425)  | 1:132:A:VAL:H    | 1:126:A:LEU:CB   | 9        | 0.35          |
| (2,369)  | 1:96:A:GLN:CB    | 1:38:A:PRO:CB    | 15       | 0.35          |
| (2,369)  | 1:96:A:GLN:CB    | 1:38:A:PRO:CB    | 17       | 0.35          |
| (2,188)  | 1:125:A:ILE:CB   | 1:23:A:LYS:CB    | 17       | 0.35          |
| (1,1241) | 1:130:A:TYR:H    | 1:127:A:PRO:HB3  | 4        | 0.35          |
| (1,1211) | 1:43:A:GLY:H     | 1:72:A:LEU:HB3   | 19       | 0.35          |
| (1,1016) | 1:126:A:LEU:H    | 1:125:A:ILE:HG12 | 1        | 0.35          |
| (1,944)  | 1:70:A:TYR:HB2   | 1:76:A:PRO:HD3   | 8        | 0.35          |
| (1,839)  | 1:6:A:HIS:H      | 1:5:A:PRO:HG3    | 9        | 0.35          |
| (1,720)  | 1:70:A:TYR:H     | 1:31:A:PRO:HG2   | 14       | 0.35          |
| (1,712)  | 1:68:A:TYR:H     | 1:48:A:HIS:H     | 10       | 0.35          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,533)  | 1:10:A:PHE:HB3  | 1:11:A:SER:HA    | 11       | 0.35          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1   | 18       | 0.35          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2   | 18       | 0.35          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2   | 15       | 0.35          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3   | 2        | 0.35          |
| (1,201)  | 1:138:A:SER:H   | 1:137:A:ARG:HB2  | 4        | 0.35          |
| (1,201)  | 1:138:A:SER:H   | 1:137:A:ARG:HB2  | 9        | 0.35          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3   | 1        | 0.35          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2   | 11       | 0.35          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2   | 14       | 0.35          |
| (1,127)  | 1:9:A:TRP:HA    | 1:71:A:TYR:HE1   | 17       | 0.35          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22   | 6        | 0.35          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21   | 6        | 0.35          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22   | 9        | 0.35          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21   | 9        | 0.35          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22   | 13       | 0.35          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21   | 13       | 0.35          |
| (1,110)  | 1:32:A:ILE:HG23 | 1:121:A:PRO:HG2  | 6        | 0.35          |
| (1,104)  | 1:108:A:ARG:H   | 1:106:A:SER:HA   | 4        | 0.35          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB   | 2        | 0.34          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB   | 12       | 0.34          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 17       | 0.34          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB     | 3        | 0.34          |
| (2,697)  | 1:119:A:ARG:H   | 1:31:A:PRO:CB    | 1        | 0.34          |
| (2,689)  | 1:106:A:SER:H   | 1:9:A:TRP:CB     | 19       | 0.34          |
| (2,654)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB   | 5        | 0.34          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB    | 12       | 0.34          |
| (2,606)  | 1:32:A:ILE:CB   | 1:34:A:PHE:H     | 6        | 0.34          |
| (2,571)  | 1:89:A:VAL:CB   | 1:45:A:TRP:CB    | 4        | 0.34          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB    | 18       | 0.34          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB    | 18       | 0.34          |
| (2,440)  | 1:91:A:TRP:H    | 1:89:A:VAL:CB    | 17       | 0.34          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 6        | 0.34          |
| (2,425)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB   | 13       | 0.34          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB    | 1        | 0.34          |
| (2,263)  | 1:16:A:PHE:CA   | 1:64:A:LEU:CB    | 4        | 0.34          |
| (2,164)  | 1:69:A:PHE:CB   | 1:10:A:PHE:CB    | 19       | 0.34          |
| (2,81)   | 1:9:A:TRP:CB    | 1:71:A:TYR:CB    | 10       | 0.34          |
| (2,56)   | 1:20:A:ARG:CB   | 1:128:A:GLN:CB   | 10       | 0.34          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2   | 8        | 0.34          |
| (1,1103) | 1:55:A:THR:H    | 1:54:A:LYS:HD3   | 7        | 0.34          |
| (1,1016) | 1:126:A:LEU:H   | 1:125:A:ILE:HG12 | 9        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1016) | 1:126:A:LEU:H    | 1:125:A:ILE:HG12 | 16       | 0.34          |
| (1,1011) | 1:42:A:LYS:HG2   | 1:72:A:LEU:HG    | 10       | 0.34          |
| (1,970)  | 1:4:A:ILE:HB     | 1:6:A:HIS:HD2    | 3        | 0.34          |
| (1,937)  | 1:69:A:PHE:HB2   | 1:31:A:PRO:HG2   | 5        | 0.34          |
| (1,839)  | 1:6:A:HIS:H      | 1:5:A:PRO:HG3    | 5        | 0.34          |
| (1,839)  | 1:6:A:HIS:H      | 1:5:A:PRO:HG3    | 18       | 0.34          |
| (1,725)  | 1:72:A:LEU:H     | 1:102:A:PRO:HA   | 6        | 0.34          |
| (1,720)  | 1:70:A:TYR:H     | 1:31:A:PRO:HG2   | 2        | 0.34          |
| (1,601)  | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD23  | 12       | 0.34          |
| (1,533)  | 1:10:A:PHE:HB3   | 1:11:A:SER:HA    | 12       | 0.34          |
| (1,359)  | 1:72:A:LEU:H     | 1:71:A:TYR:HB2   | 13       | 0.34          |
| (1,324)  | 1:73:A:GLY:H     | 1:74:A:THR:HB    | 14       | 0.34          |
| (1,263)  | 1:82:A:TYR:HA    | 1:83:A:GLY:H     | 6        | 0.34          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3   | 11       | 0.34          |
| (1,124)  | 1:5:A:PRO:HD3    | 1:4:A:ILE:HG22   | 4        | 0.34          |
| (1,124)  | 1:5:A:PRO:HD3    | 1:4:A:ILE:HG21   | 4        | 0.34          |
| (1,78)   | 1:82:A:TYR:HB2   | 1:83:A:GLY:HA2   | 3        | 0.34          |
| (1,54)   | 1:63:A:LEU:HA    | 1:62:A:GLN:HG2   | 14       | 0.34          |
| (2,1200) | 1:130:A:TYR:CB   | 1:126:A:LEU:CB   | 18       | 0.33          |
| (2,1102) | 1:130:A:TYR:H    | 1:17:A:GLN:CB    | 13       | 0.33          |
| (2,1099) | 1:120:A:PHE:H    | 1:32:A:ILE:CB    | 2        | 0.33          |
| (2,854)  | 1:14:A:THR:CA    | 1:66:A:ARG:CB    | 4        | 0.33          |
| (2,850)  | 1:5:A:PRO:CB     | 1:6:A:HIS:CB     | 4        | 0.33          |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 14       | 0.33          |
| (2,817)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 14       | 0.33          |
| (2,802)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 19       | 0.33          |
| (2,802)  | 1:132:A:VAL:CB   | 1:126:A:LEU:CB   | 19       | 0.33          |
| (2,727)  | 1:114:A:GLU:CB   | 1:116:A:ILE:CB   | 6        | 0.33          |
| (2,718)  | 1:42:A:LYS:H     | 1:40:A:GLU:CB    | 7        | 0.33          |
| (2,645)  | 1:68:A:TYR:H     | 1:69:A:PHE:CB    | 7        | 0.33          |
| (2,440)  | 1:91:A:TRP:H     | 1:89:A:VAL:CB    | 8        | 0.33          |
| (2,356)  | 1:31:A:PRO:CB    | 1:120:A:PHE:CB   | 16       | 0.33          |
| (1,1016) | 1:126:A:LEU:H    | 1:125:A:ILE:HG12 | 4        | 0.33          |
| (1,937)  | 1:69:A:PHE:HB2   | 1:31:A:PRO:HG2   | 6        | 0.33          |
| (1,937)  | 1:69:A:PHE:HB2   | 1:31:A:PRO:HG2   | 17       | 0.33          |
| (1,839)  | 1:6:A:HIS:H      | 1:5:A:PRO:HG3    | 14       | 0.33          |
| (1,807)  | 1:116:A:ILE:HG22 | 1:117:A:PRO:HD3  | 8        | 0.33          |
| (1,807)  | 1:116:A:ILE:HG21 | 1:117:A:PRO:HD3  | 8        | 0.33          |
| (1,680)  | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 14       | 0.33          |
| (1,601)  | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD23  | 16       | 0.33          |
| (1,384)  | 1:31:A:PRO:HB3   | 1:10:A:PHE:HE1   | 6        | 0.33          |
| (1,384)  | 1:31:A:PRO:HB3   | 1:10:A:PHE:HE2   | 6        | 0.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2   | 11       | 0.33          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2   | 18       | 0.33          |
| (1,343)  | 1:97:A:ALA:H    | 1:39:A:SER:HA    | 18       | 0.33          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3   | 9        | 0.33          |
| (1,288)  | 1:16:A:PHE:HA   | 1:64:A:LEU:HD23  | 7        | 0.33          |
| (1,277)  | 1:111:A:THR:H   | 1:110:A:PRO:HB3  | 7        | 0.33          |
| (1,263)  | 1:82:A:TYR:HA   | 1:83:A:GLY:H     | 13       | 0.33          |
| (1,263)  | 1:82:A:TYR:HA   | 1:83:A:GLY:H     | 16       | 0.33          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2   | 2        | 0.33          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2   | 9        | 0.33          |
| (1,104)  | 1:108:A:ARG:H   | 1:106:A:SER:HA   | 3        | 0.33          |
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB    | 18       | 0.32          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB    | 7        | 0.32          |
| (2,1102) | 1:130:A:TYR:H   | 1:17:A:GLN:CB    | 14       | 0.32          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 12       | 0.32          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB    | 14       | 0.32          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB    | 19       | 0.32          |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB   | 19       | 0.32          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB   | 16       | 0.32          |
| (2,850)  | 1:5:A:PRO:CB    | 1:6:A:HIS:CB     | 19       | 0.32          |
| (2,697)  | 1:119:A:ARG:H   | 1:31:A:PRO:CB    | 19       | 0.32          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB    | 14       | 0.32          |
| (2,440)  | 1:91:A:TRP:H    | 1:89:A:VAL:CB    | 11       | 0.32          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 19       | 0.32          |
| (2,425)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB   | 2        | 0.32          |
| (2,385)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB    | 5        | 0.32          |
| (2,369)  | 1:96:A:GLN:CB   | 1:38:A:PRO:CB    | 7        | 0.32          |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB    | 14       | 0.32          |
| (2,68)   | 1:86:A:LEU:H    | 1:45:A:TRP:CB    | 4        | 0.32          |
| (2,68)   | 1:86:A:LEU:H    | 1:45:A:TRP:CB    | 19       | 0.32          |
| (2,24)   | 1:60:A:GLN:CB   | 1:54:A:LYS:CB    | 18       | 0.32          |
| (2,23)   | 1:115:A:ALA:H   | 1:114:A:GLU:CB   | 18       | 0.32          |
| (1,1154) | 1:11:A:SER:HA   | 1:136:A:GLY:HA3  | 5        | 0.32          |
| (1,1016) | 1:126:A:LEU:H   | 1:125:A:ILE:HG12 | 15       | 0.32          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2    | 8        | 0.32          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2    | 11       | 0.32          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2    | 16       | 0.32          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2   | 10       | 0.32          |
| (1,909)  | 1:117:A:PRO:HA  | 1:134:A:GLY:HA2  | 16       | 0.32          |
| (1,856)  | 1:81:A:SER:HB2  | 1:82:A:TYR:HA    | 6        | 0.32          |
| (1,856)  | 1:81:A:SER:HB2  | 1:82:A:TYR:HA    | 16       | 0.32          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2  | 19       | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 8        | 0.32          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 16       | 0.32          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 15       | 0.32          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 8        | 0.32          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 11       | 0.32          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 6        | 0.32          |
| (1,411)  | 1:16:A:PHE:H    | 1:64:A:LEU:HB3  | 5        | 0.32          |
| (1,402)  | 1:32:A:ILE:HD12 | 1:121:A:PRO:HG2 | 11       | 0.32          |
| (1,402)  | 1:32:A:ILE:HD11 | 1:121:A:PRO:HG2 | 11       | 0.32          |
| (1,402)  | 1:32:A:ILE:HD13 | 1:121:A:PRO:HG2 | 11       | 0.32          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1  | 14       | 0.32          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2  | 14       | 0.32          |
| (1,324)  | 1:73:A:GLY:H    | 1:74:A:THR:HB   | 18       | 0.32          |
| (1,281)  | 1:109:A:ASP:H   | 1:108:A:ARG:HB3 | 3        | 0.32          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 10       | 0.32          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 10       | 0.32          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 19       | 0.32          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 19       | 0.32          |
| (1,104)  | 1:108:A:ARG:H   | 1:106:A:SER:HA  | 8        | 0.32          |
| (1,33)   | 1:16:A:PHE:H    | 1:17:A:GLN:HB2  | 7        | 0.32          |
| (1,6)    | 1:44:A:TYR:H    | 1:91:A:TRP:HZ3  | 8        | 0.32          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 14       | 0.31          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 3        | 0.31          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 13       | 0.31          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 15       | 0.31          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 14       | 0.31          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 8        | 0.31          |
| (2,762)  | 1:126:A:LEU:H   | 1:127:A:PRO:CB  | 17       | 0.31          |
| (2,718)  | 1:42:A:LYS:H    | 1:40:A:GLU:CB   | 2        | 0.31          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB   | 13       | 0.31          |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 7        | 0.31          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 17       | 0.31          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 17       | 0.31          |
| (2,481)  | 1:118:A:THR:H   | 1:11:A:SER:H    | 13       | 0.31          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 16       | 0.31          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 16       | 0.31          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 7        | 0.31          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB   | 19       | 0.31          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 2        | 0.31          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 7        | 0.31          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 15       | 0.31          |
| (2,338)  | 1:66:A:ARG:H    | 1:48:A:HIS:CB   | 10       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,261)  | 1:108:A:ARG:H    | 1:107:A:SER:H    | 17       | 0.31          |
| (2,255)  | 1:112:A:THR:H    | 1:109:A:ASP:H    | 12       | 0.31          |
| (2,240)  | 1:20:A:ARG:H     | 1:17:A:GLN:CB    | 10       | 0.31          |
| (2,102)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB    | 4        | 0.31          |
| (1,1241) | 1:130:A:TYR:H    | 1:127:A:PRO:HB3  | 17       | 0.31          |
| (1,1128) | 1:73:A:GLY:HA3   | 1:102:A:PRO:HG2  | 5        | 0.31          |
| (1,1029) | 1:51:A:ARG:HA    | 1:63:A:LEU:HD21  | 10       | 0.31          |
| (1,1016) | 1:126:A:LEU:H    | 1:125:A:ILE:HG12 | 3        | 0.31          |
| (1,847)  | 1:122:A:PRO:HD2  | 1:121:A:PRO:HB2  | 16       | 0.31          |
| (1,785)  | 1:113:A:GLN:HG2  | 1:110:A:PRO:HB2  | 13       | 0.31          |
| (1,601)  | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD23  | 5        | 0.31          |
| (1,601)  | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD23  | 13       | 0.31          |
| (1,521)  | 1:118:A:THR:H    | 1:11:A:SER:H     | 13       | 0.31          |
| (1,517)  | 1:43:A:GLY:HA2   | 1:70:A:TYR:HA    | 1        | 0.31          |
| (1,364)  | 1:82:A:TYR:H     | 1:83:A:GLY:H     | 2        | 0.31          |
| (1,364)  | 1:82:A:TYR:H     | 1:83:A:GLY:H     | 7        | 0.31          |
| (1,364)  | 1:82:A:TYR:H     | 1:83:A:GLY:H     | 15       | 0.31          |
| (1,359)  | 1:72:A:LEU:H     | 1:71:A:TYR:HB2   | 1        | 0.31          |
| (1,359)  | 1:72:A:LEU:H     | 1:71:A:TYR:HB2   | 4        | 0.31          |
| (1,324)  | 1:73:A:GLY:H     | 1:74:A:THR:HB    | 15       | 0.31          |
| (1,292)  | 1:17:A:GLN:H     | 1:16:A:PHE:HB3   | 12       | 0.31          |
| (1,284)  | 1:108:A:ARG:H    | 1:107:A:SER:H    | 17       | 0.31          |
| (1,276)  | 1:112:A:THR:H    | 1:109:A:ASP:H    | 12       | 0.31          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3   | 13       | 0.31          |
| (1,173)  | 1:36:A:VAL:H     | 1:35:A:GLY:HA2   | 13       | 0.31          |
| (1,155)  | 1:106:A:SER:H    | 1:105:A:VAL:HA   | 4        | 0.31          |
| (1,124)  | 1:5:A:PRO:HD3    | 1:4:A:ILE:HG22   | 3        | 0.31          |
| (1,124)  | 1:5:A:PRO:HD3    | 1:4:A:ILE:HG21   | 3        | 0.31          |
| (1,110)  | 1:32:A:ILE:HG23  | 1:121:A:PRO:HG2  | 8        | 0.31          |
| (1,33)   | 1:16:A:PHE:H     | 1:17:A:GLN:HB2   | 6        | 0.31          |
| (2,1200) | 1:130:A:TYR:CB   | 1:126:A:LEU:CB   | 9        | 0.3           |
| (2,1138) | 1:103:A:SER:CA   | 1:42:A:LYS:CB    | 14       | 0.3           |
| (2,1138) | 1:103:A:SER:CA   | 1:42:A:LYS:CB    | 16       | 0.3           |
| (2,1059) | 1:48:A:HIS:H     | 1:46:A:TYR:CB    | 13       | 0.3           |
| (2,891)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB    | 16       | 0.3           |
| (2,718)  | 1:42:A:LYS:H     | 1:40:A:GLU:CB    | 3        | 0.3           |
| (2,718)  | 1:42:A:LYS:H     | 1:40:A:GLU:CB    | 5        | 0.3           |
| (2,645)  | 1:68:A:TYR:H     | 1:69:A:PHE:CB    | 5        | 0.3           |
| (2,645)  | 1:68:A:TYR:H     | 1:69:A:PHE:CB    | 10       | 0.3           |
| (2,645)  | 1:68:A:TYR:H     | 1:69:A:PHE:CB    | 19       | 0.3           |
| (2,537)  | 1:124:A:THR:H    | 1:28:A:GLN:CB    | 12       | 0.3           |
| (2,440)  | 1:91:A:TRP:H     | 1:89:A:VAL:CB    | 14       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,369)  | 1:96:A:GLN:CB   | 1:38:A:PRO:CB   | 13       | 0.3           |
| (2,358)  | 1:31:A:PRO:CB   | 1:10:A:PHE:CB   | 7        | 0.3           |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 15       | 0.3           |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 9        | 0.3           |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 14       | 0.3           |
| (2,102)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 3        | 0.3           |
| (2,81)   | 1:9:A:TRP:CB    | 1:71:A:TYR:CB   | 15       | 0.3           |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB   | 2        | 0.3           |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 12       | 0.3           |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 13       | 0.3           |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 13       | 0.3           |
| (1,1242) | 1:130:A:TYR:H   | 1:17:A:GLN:HB2  | 5        | 0.3           |
| (1,1211) | 1:43:A:GLY:H    | 1:72:A:LEU:HB3  | 10       | 0.3           |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 1        | 0.3           |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE2  | 1        | 0.3           |
| (1,1038) | 1:60:A:GLN:HB3  | 1:54:A:LYS:HE3  | 1        | 0.3           |
| (1,1017) | 1:29:A:GLY:H    | 1:28:A:GLN:HB3  | 18       | 0.3           |
| (1,955)  | 1:13:A:ILE:HA   | 1:66:A:ARG:HG2  | 13       | 0.3           |
| (1,856)  | 1:81:A:SER:HB2  | 1:82:A:TYR:HA   | 13       | 0.3           |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 17       | 0.3           |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 7        | 0.3           |
| (1,595)  | 1:115:A:ALA:HA  | 1:114:A:GLU:HB2 | 16       | 0.3           |
| (1,533)  | 1:10:A:PHE:HB3  | 1:11:A:SER:HA   | 3        | 0.3           |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 9        | 0.3           |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 14       | 0.3           |
| (1,343)  | 1:97:A:ALA:H    | 1:39:A:SER:HA   | 15       | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 7        | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 7        | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 8        | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 8        | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 11       | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 11       | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 12       | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 12       | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 18       | 0.3           |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 18       | 0.3           |
| (1,110)  | 1:32:A:ILE:HG23 | 1:121:A:PRO:HG2 | 9        | 0.3           |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2 | 16       | 0.3           |
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB   | 4        | 0.29          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB  | 14       | 0.29          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 1        | 0.29          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 11       | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB    | 15       | 0.29          |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB   | 7        | 0.29          |
| (2,885)  | 1:32:A:ILE:CB   | 1:120:A:PHE:CB   | 10       | 0.29          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 7        | 0.29          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 7        | 0.29          |
| (2,792)  | 1:108:A:ARG:H   | 1:9:A:TRP:CB     | 8        | 0.29          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB    | 2        | 0.29          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB    | 17       | 0.29          |
| (2,564)  | 1:127:A:PRO:CB  | 1:23:A:LYS:CB    | 2        | 0.29          |
| (2,560)  | 1:84:A:GLU:H    | 1:91:A:TRP:CB    | 11       | 0.29          |
| (2,440)  | 1:91:A:TRP:H    | 1:89:A:VAL:CB    | 6        | 0.29          |
| (2,404)  | 1:71:A:TYR:H    | 1:74:A:THR:CB    | 1        | 0.29          |
| (2,404)  | 1:71:A:TYR:H    | 1:74:A:THR:CB    | 13       | 0.29          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 6        | 0.29          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 3        | 0.29          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 4        | 0.29          |
| (2,261)  | 1:108:A:ARG:H   | 1:107:A:SER:H    | 9        | 0.29          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3  | 12       | 0.29          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H     | 4        | 0.29          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2    | 15       | 0.29          |
| (1,950)  | 1:8:A:SER:HB2   | 1:7:A:TYR:HA     | 17       | 0.29          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2   | 15       | 0.29          |
| (1,924)  | 1:71:A:TYR:HD2  | 1:105:A:VAL:HG23 | 14       | 0.29          |
| (1,849)  | 1:25:A:SER:H    | 1:28:A:GLN:HB3   | 18       | 0.29          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3    | 15       | 0.29          |
| (1,768)  | 1:119:A:ARG:H   | 1:31:A:PRO:HB3   | 19       | 0.29          |
| (1,631)  | 1:89:A:VAL:HG23 | 1:86:A:LEU:HB3   | 5        | 0.29          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3   | 13       | 0.29          |
| (1,385)  | 1:118:A:THR:H   | 1:117:A:PRO:HB2  | 16       | 0.29          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12  | 4        | 0.29          |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 3        | 0.29          |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 4        | 0.29          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3   | 4        | 0.29          |
| (1,284)  | 1:108:A:ARG:H   | 1:107:A:SER:H    | 9        | 0.29          |
| (1,281)  | 1:109:A:ASP:H   | 1:108:A:ARG:HB3  | 13       | 0.29          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2   | 6        | 0.29          |
| (1,155)  | 1:106:A:SER:H   | 1:105:A:VAL:HA   | 14       | 0.29          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22   | 5        | 0.29          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21   | 5        | 0.29          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22   | 14       | 0.29          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21   | 14       | 0.29          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22   | 15       | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21   | 15       | 0.29          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22   | 16       | 0.29          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21   | 16       | 0.29          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2   | 19       | 0.29          |
| (1,53)   | 1:138:A:SER:HA  | 1:11:A:SER:HB3   | 4        | 0.29          |
| (1,33)   | 1:16:A:PHE:H    | 1:17:A:GLN:HB2   | 8        | 0.29          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB   | 8        | 0.28          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB    | 2        | 0.28          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB    | 17       | 0.28          |
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 14       | 0.28          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB    | 9        | 0.28          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB    | 17       | 0.28          |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB   | 14       | 0.28          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 8        | 0.28          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 8        | 0.28          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 15       | 0.28          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB   | 15       | 0.28          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB    | 8        | 0.28          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB    | 3        | 0.28          |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB    | 1        | 0.28          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB    | 12       | 0.28          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB    | 12       | 0.28          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB    | 19       | 0.28          |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB    | 19       | 0.28          |
| (2,444)  | 1:104:A:ASP:CB  | 1:36:A:VAL:CB    | 13       | 0.28          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 18       | 0.28          |
| (2,261)  | 1:108:A:ARG:H   | 1:107:A:SER:H    | 3        | 0.28          |
| (2,261)  | 1:108:A:ARG:H   | 1:107:A:SER:H    | 8        | 0.28          |
| (2,78)   | 1:44:A:TYR:CB   | 1:77:A:TYR:CB    | 4        | 0.28          |
| (2,33)   | 1:104:A:ASP:H   | 1:105:A:VAL:CB   | 9        | 0.28          |
| (1,1294) | 1:63:A:LEU:HG   | 1:61:A:LYS:HG3   | 1        | 0.28          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3   | 5        | 0.28          |
| (1,1241) | 1:130:A:TYR:H   | 1:127:A:PRO:HB3  | 7        | 0.28          |
| (1,1241) | 1:130:A:TYR:H   | 1:127:A:PRO:HB3  | 19       | 0.28          |
| (1,1128) | 1:73:A:GLY:HA3  | 1:102:A:PRO:HG2  | 11       | 0.28          |
| (1,1103) | 1:55:A:THR:H    | 1:54:A:LYS:HD3   | 6        | 0.28          |
| (1,1016) | 1:126:A:LEU:H   | 1:125:A:ILE:HG12 | 13       | 0.28          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2    | 2        | 0.28          |
| (1,794)  | 1:114:A:GLU:HG2 | 1:115:A:ALA:HB2  | 6        | 0.28          |
| (1,794)  | 1:114:A:GLU:HG2 | 1:115:A:ALA:HB1  | 6        | 0.28          |
| (1,794)  | 1:114:A:GLU:HG2 | 1:115:A:ALA:HB3  | 6        | 0.28          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA   | 5        | 0.28          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,605)  | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 5        | 0.28          |
| (1,601)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD23 | 6        | 0.28          |
| (1,599)  | 1:84:A:GLU:HB2 | 1:86:A:LEU:HD22 | 2        | 0.28          |
| (1,359)  | 1:72:A:LEU:H   | 1:71:A:TYR:HB2  | 6        | 0.28          |
| (1,343)  | 1:97:A:ALA:H   | 1:39:A:SER:HA   | 8        | 0.28          |
| (1,302)  | 1:43:A:GLY:HA3 | 1:72:A:LEU:H    | 19       | 0.28          |
| (1,292)  | 1:17:A:GLN:H   | 1:16:A:PHE:HB3  | 3        | 0.28          |
| (1,284)  | 1:108:A:ARG:H  | 1:107:A:SER:H   | 3        | 0.28          |
| (1,284)  | 1:108:A:ARG:H  | 1:107:A:SER:H   | 8        | 0.28          |
| (1,173)  | 1:36:A:VAL:H   | 1:35:A:GLY:HA2  | 15       | 0.28          |
| (1,78)   | 1:82:A:TYR:HB2 | 1:83:A:GLY:HA2  | 9        | 0.28          |
| (1,33)   | 1:16:A:PHE:H   | 1:17:A:GLN:HB2  | 2        | 0.28          |
| (1,33)   | 1:16:A:PHE:H   | 1:17:A:GLN:HB2  | 4        | 0.28          |
| (1,33)   | 1:16:A:PHE:H   | 1:17:A:GLN:HB2  | 12       | 0.28          |
| (1,33)   | 1:16:A:PHE:H   | 1:17:A:GLN:HB2  | 13       | 0.28          |
| (2,1138) | 1:103:A:SER:CA | 1:42:A:LYS:CB   | 3        | 0.27          |
| (2,1138) | 1:103:A:SER:CA | 1:42:A:LYS:CB   | 6        | 0.27          |
| (2,1138) | 1:103:A:SER:CA | 1:42:A:LYS:CB   | 17       | 0.27          |
| (2,1066) | 1:108:A:ARG:CA | 1:9:A:TRP:CB    | 5        | 0.27          |
| (2,945)  | 1:22:A:PHE:CA  | 1:127:A:PRO:CB  | 8        | 0.27          |
| (2,775)  | 1:28:A:GLN:H   | 1:25:A:SER:CB   | 19       | 0.27          |
| (2,718)  | 1:42:A:LYS:H   | 1:40:A:GLU:CB   | 1        | 0.27          |
| (2,645)  | 1:68:A:TYR:H   | 1:69:A:PHE:CB   | 8        | 0.27          |
| (2,645)  | 1:68:A:TYR:H   | 1:69:A:PHE:CB   | 15       | 0.27          |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB   | 1        | 0.27          |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB   | 4        | 0.27          |
| (2,623)  | 1:99:A:THR:CA  | 1:42:A:LYS:CB   | 11       | 0.27          |
| (2,551)  | 1:20:A:ARG:H   | 1:17:A:GLN:CB   | 1        | 0.27          |
| (2,537)  | 1:124:A:THR:H  | 1:28:A:GLN:CB   | 5        | 0.27          |
| (2,526)  | 1:39:A:SER:H   | 1:96:A:GLN:CB   | 15       | 0.27          |
| (2,526)  | 1:39:A:SER:H   | 1:96:A:GLN:CB   | 15       | 0.27          |
| (2,466)  | 1:41:A:ALA:CA  | 1:30:A:VAL:CB   | 11       | 0.27          |
| (2,440)  | 1:91:A:TRP:H   | 1:89:A:VAL:CB   | 12       | 0.27          |
| (2,436)  | 1:33:A:ALA:CB  | 1:36:A:VAL:CB   | 4        | 0.27          |
| (2,369)  | 1:96:A:GLN:CB  | 1:38:A:PRO:CB   | 9        | 0.27          |
| (2,339)  | 1:82:A:TYR:H   | 1:83:A:GLY:H    | 12       | 0.27          |
| (2,130)  | 1:120:A:PHE:CB | 1:30:A:VAL:CA   | 17       | 0.27          |
| (2,78)   | 1:44:A:TYR:CB  | 1:77:A:TYR:CB   | 6        | 0.27          |
| (2,23)   | 1:115:A:ALA:H  | 1:114:A:GLU:CB  | 2        | 0.27          |
| (1,1294) | 1:63:A:LEU:HG  | 1:61:A:LYS:HG3  | 9        | 0.27          |
| (1,1256) | 1:27:A:GLY:H   | 1:28:A:GLN:HB3  | 7        | 0.27          |
| (1,1041) | 1:57:A:ASP:HA  | 1:58:A:GLY:H    | 6        | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 7        | 0.27          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2   | 5        | 0.27          |
| (1,952)  | 1:6:A:HIS:HD2   | 1:4:A:ILE:HG22  | 1        | 0.27          |
| (1,952)  | 1:6:A:HIS:HD2   | 1:4:A:ILE:HG21  | 1        | 0.27          |
| (1,887)  | 1:129:A:GLY:HA3 | 1:128:A:GLN:HG3 | 10       | 0.27          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 3        | 0.27          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 4        | 0.27          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 3        | 0.27          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 12       | 0.27          |
| (1,788)  | 1:20:A:ARG:HB3  | 1:17:A:GLN:HE22 | 1        | 0.27          |
| (1,720)  | 1:70:A:TYR:H    | 1:31:A:PRO:HG2  | 15       | 0.27          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 10       | 0.27          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 13       | 0.27          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 8        | 0.27          |
| (1,385)  | 1:118:A:THR:H   | 1:117:A:PRO:HB2 | 7        | 0.27          |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 12       | 0.27          |
| (1,343)  | 1:97:A:ALA:H    | 1:39:A:SER:HA   | 2        | 0.27          |
| (1,324)  | 1:73:A:GLY:H    | 1:74:A:THR:HB   | 17       | 0.27          |
| (1,192)  | 1:25:A:SER:H    | 1:24:A:PHE:HB3  | 18       | 0.27          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2  | 5        | 0.27          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2  | 7        | 0.27          |
| (1,78)   | 1:82:A:TYR:HB2  | 1:83:A:GLY:HA2  | 4        | 0.27          |
| (1,78)   | 1:82:A:TYR:HB2  | 1:83:A:GLY:HA2  | 12       | 0.27          |
| (1,33)   | 1:16:A:PHE:H    | 1:17:A:GLN:HB2  | 9        | 0.27          |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2 | 18       | 0.27          |
| (2,1156) | 1:98:A:ASP:CA   | 1:42:A:LYS:CB   | 12       | 0.26          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 12       | 0.26          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 13       | 0.26          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB   | 18       | 0.26          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 3        | 0.26          |
| (2,885)  | 1:32:A:ILE:CB   | 1:120:A:PHE:CB  | 19       | 0.26          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 19       | 0.26          |
| (2,817)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 19       | 0.26          |
| (2,676)  | 1:113:A:GLN:CB  | 1:112:A:THR:CB  | 13       | 0.26          |
| (2,654)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 14       | 0.26          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB   | 18       | 0.26          |
| (2,571)  | 1:89:A:VAL:CB   | 1:45:A:TRP:CB   | 3        | 0.26          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 7        | 0.26          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 7        | 0.26          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 13       | 0.26          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 13       | 0.26          |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB   | 1        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 4        | 0.26          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 5        | 0.26          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 10       | 0.26          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 3        | 0.26          |
| (2,152)  | 1:7:A:TYR:CB    | 1:110:A:PRO:CB  | 10       | 0.26          |
| (2,128)  | 1:28:A:GLN:CA   | 1:120:A:PHE:CB  | 7        | 0.26          |
| (2,128)  | 1:28:A:GLN:CA   | 1:120:A:PHE:CB  | 9        | 0.26          |
| (2,68)   | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 3        | 0.26          |
| (2,68)   | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 6        | 0.26          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 13       | 0.26          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 17       | 0.26          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 3        | 0.26          |
| (1,1334) | 1:16:A:PHE:HB3  | 1:130:A:TYR:HB3 | 8        | 0.26          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 18       | 0.26          |
| (1,1272) | 1:129:A:GLY:HA3 | 1:17:A:GLN:HB2  | 7        | 0.26          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 3        | 0.26          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 8        | 0.26          |
| (1,1177) | 1:51:A:ARG:HB3  | 1:63:A:LEU:HD21 | 11       | 0.26          |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 13       | 0.26          |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 13       | 0.26          |
| (1,1128) | 1:73:A:GLY:HA3  | 1:102:A:PRO:HG2 | 18       | 0.26          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 14       | 0.26          |
| (1,873)  | 1:78:A:ALA:H    | 1:76:A:PRO:HD3  | 18       | 0.26          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 18       | 0.26          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 11       | 0.26          |
| (1,794)  | 1:114:A:GLU:HG2 | 1:115:A:ALA:HB2 | 15       | 0.26          |
| (1,794)  | 1:114:A:GLU:HG2 | 1:115:A:ALA:HB1 | 15       | 0.26          |
| (1,794)  | 1:114:A:GLU:HG2 | 1:115:A:ALA:HB3 | 15       | 0.26          |
| (1,785)  | 1:113:A:GLN:HG2 | 1:110:A:PRO:HB2 | 10       | 0.26          |
| (1,768)  | 1:119:A:ARG:H   | 1:31:A:PRO:HB3  | 1        | 0.26          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 13       | 0.26          |
| (1,621)  | 1:89:A:VAL:HG12 | 1:86:A:LEU:HD22 | 7        | 0.26          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3  | 15       | 0.26          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3  | 19       | 0.26          |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23 | 11       | 0.26          |
| (1,414)  | 1:65:A:PRO:HB3  | 1:67:A:TRP:HE1  | 5        | 0.26          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2  | 12       | 0.26          |
| (1,333)  | 1:81:A:SER:HA   | 1:84:A:GLU:HB3  | 16       | 0.26          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3  | 6        | 0.26          |
| (1,138)  | 1:138:A:SER:H   | 1:137:A:ARG:HA  | 5        | 0.26          |
| (1,114)  | 1:104:A:ASP:H   | 1:103:A:SER:HA  | 1        | 0.26          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2  | 1        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3  | 6        | 0.26          |
| (2,1149) | 1:18:A:LYS:CB   | 1:64:A:LEU:CB   | 14       | 0.25          |
| (2,1148) | 1:64:A:LEU:CB   | 1:18:A:LYS:CB   | 14       | 0.25          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 11       | 0.25          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 18       | 0.25          |
| (2,1126) | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 8        | 0.25          |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB  | 3        | 0.25          |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB  | 4        | 0.25          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB  | 4        | 0.25          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB  | 5        | 0.25          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 8        | 0.25          |
| (2,885)  | 1:32:A:ILE:CB   | 1:120:A:PHE:CB  | 4        | 0.25          |
| (2,783)  | 1:124:A:THR:CB  | 1:24:A:PHE:CB   | 3        | 0.25          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB   | 4        | 0.25          |
| (2,538)  | 1:13:A:ILE:H    | 1:69:A:PHE:CB   | 4        | 0.25          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 11       | 0.25          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 11       | 0.25          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 7        | 0.25          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 18       | 0.25          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB   | 16       | 0.25          |
| (2,403)  | 1:105:A:VAL:H   | 1:74:A:THR:CB   | 1        | 0.25          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 6        | 0.25          |
| (2,283)  | 1:81:A:SER:CB   | 1:84:A:GLU:CB   | 13       | 0.25          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 8        | 0.25          |
| (2,81)   | 1:9:A:TRP:CB    | 1:71:A:TYR:CB   | 12       | 0.25          |
| (2,80)   | 1:113:A:GLN:CB  | 1:9:A:TRP:CB    | 17       | 0.25          |
| (2,23)   | 1:115:A:ALA:H   | 1:114:A:GLU:CB  | 19       | 0.25          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 6        | 0.25          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 9        | 0.25          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 6        | 0.25          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 13       | 0.25          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 14       | 0.25          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 15       | 0.25          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 5        | 0.25          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2   | 18       | 0.25          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 10       | 0.25          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 9        | 0.25          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 14       | 0.25          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 15       | 0.25          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 17       | 0.25          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 15       | 0.25          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3  | 11       | 0.25          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,595)  | 1:115:A:ALA:HA   | 1:114:A:GLU:HB2 | 2        | 0.25          |
| (1,471)  | 1:84:A:GLU:H     | 1:86:A:LEU:HD23 | 18       | 0.25          |
| (1,402)  | 1:32:A:ILE:HD12  | 1:121:A:PRO:HG2 | 13       | 0.25          |
| (1,402)  | 1:32:A:ILE:HD11  | 1:121:A:PRO:HG2 | 13       | 0.25          |
| (1,402)  | 1:32:A:ILE:HD13  | 1:121:A:PRO:HG2 | 13       | 0.25          |
| (1,359)  | 1:72:A:LEU:H     | 1:71:A:TYR:HB2  | 7        | 0.25          |
| (1,359)  | 1:72:A:LEU:H     | 1:71:A:TYR:HB2  | 9        | 0.25          |
| (1,343)  | 1:97:A:ALA:H     | 1:39:A:SER:HA   | 6        | 0.25          |
| (1,324)  | 1:73:A:GLY:H     | 1:74:A:THR:HB   | 9        | 0.25          |
| (1,292)  | 1:17:A:GLN:H     | 1:16:A:PHE:HB3  | 13       | 0.25          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3  | 9        | 0.25          |
| (1,54)   | 1:63:A:LEU:HA    | 1:62:A:GLN:HG2  | 13       | 0.25          |
| (2,1138) | 1:103:A:SER:CA   | 1:42:A:LYS:CB   | 10       | 0.24          |
| (2,1112) | 1:121:A:PRO:CA   | 1:32:A:ILE:CB   | 6        | 0.24          |
| (2,1102) | 1:130:A:TYR:H    | 1:17:A:GLN:CB   | 5        | 0.24          |
| (2,1102) | 1:130:A:TYR:H    | 1:17:A:GLN:CB   | 16       | 0.24          |
| (2,1059) | 1:48:A:HIS:H     | 1:46:A:TYR:CB   | 17       | 0.24          |
| (2,956)  | 1:9:A:TRP:CB     | 1:107:A:SER:CB  | 4        | 0.24          |
| (2,945)  | 1:22:A:PHE:CA    | 1:127:A:PRO:CB  | 6        | 0.24          |
| (2,929)  | 1:60:A:GLN:CB    | 1:54:A:LYS:CB   | 18       | 0.24          |
| (2,926)  | 1:101:A:THR:CB   | 1:100:A:SER:CB  | 13       | 0.24          |
| (2,718)  | 1:42:A:LYS:H     | 1:40:A:GLU:CB   | 9        | 0.24          |
| (2,718)  | 1:42:A:LYS:H     | 1:40:A:GLU:CB   | 17       | 0.24          |
| (2,645)  | 1:68:A:TYR:H     | 1:69:A:PHE:CB   | 1        | 0.24          |
| (2,469)  | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 17       | 0.24          |
| (2,440)  | 1:91:A:TRP:H     | 1:89:A:VAL:CB   | 10       | 0.24          |
| (2,428)  | 1:132:A:VAL:H    | 1:126:A:LEU:CB  | 19       | 0.24          |
| (2,426)  | 1:40:A:GLU:H     | 1:36:A:VAL:CB   | 19       | 0.24          |
| (2,403)  | 1:105:A:VAL:H    | 1:74:A:THR:CB   | 8        | 0.24          |
| (2,356)  | 1:31:A:PRO:CB    | 1:120:A:PHE:CB  | 12       | 0.24          |
| (2,352)  | 1:31:A:PRO:CA    | 1:10:A:PHE:CB   | 12       | 0.24          |
| (2,241)  | 1:101:A:THR:CB   | 1:100:A:SER:CB  | 13       | 0.24          |
| (2,74)   | 1:13:A:ILE:CA    | 1:133:A:GLU:H   | 1        | 0.24          |
| (2,33)   | 1:104:A:ASP:H    | 1:105:A:VAL:CB  | 4        | 0.24          |
| (2,33)   | 1:104:A:ASP:H    | 1:105:A:VAL:CB  | 18       | 0.24          |
| (2,3)    | 1:46:A:TYR:CB    | 1:76:A:PRO:CB   | 5        | 0.24          |
| (1,1272) | 1:129:A:GLY:HA3  | 1:17:A:GLN:HB2  | 3        | 0.24          |
| (1,1272) | 1:129:A:GLY:HA3  | 1:17:A:GLN:HB2  | 15       | 0.24          |
| (1,1267) | 1:51:A:ARG:HB2   | 1:63:A:LEU:HD23 | 1        | 0.24          |
| (1,1256) | 1:27:A:GLY:H     | 1:28:A:GLN:HB3  | 14       | 0.24          |
| (1,1174) | 1:51:A:ARG:HB2   | 1:63:A:LEU:HD23 | 1        | 0.24          |
| (1,1167) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2  | 2        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 2        | 0.24          |
| (1,1104) | 1:52:A:SER:HA   | 1:51:A:ARG:HG2  | 15       | 0.24          |
| (1,1014) | 1:62:A:GLN:HA   | 1:52:A:SER:HA   | 3        | 0.24          |
| (1,970)  | 1:4:A:ILE:HB    | 1:6:A:HIS:HD2   | 12       | 0.24          |
| (1,955)  | 1:13:A:ILE:HA   | 1:66:A:ARG:HG2  | 17       | 0.24          |
| (1,887)  | 1:129:A:GLY:HA3 | 1:128:A:GLN:HG3 | 5        | 0.24          |
| (1,874)  | 1:126:A:LEU:HB2 | 1:127:A:PRO:HD3 | 7        | 0.24          |
| (1,874)  | 1:126:A:LEU:HB2 | 1:127:A:PRO:HD3 | 19       | 0.24          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 15       | 0.24          |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 7        | 0.24          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 4        | 0.24          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 6        | 0.24          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3   | 17       | 0.24          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3  | 6        | 0.24          |
| (1,595)  | 1:115:A:ALA:HA  | 1:114:A:GLU:HB2 | 18       | 0.24          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 10       | 0.24          |
| (1,509)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 17       | 0.24          |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23 | 2        | 0.24          |
| (1,385)  | 1:118:A:THR:H   | 1:117:A:PRO:HB2 | 12       | 0.24          |
| (1,385)  | 1:118:A:THR:H   | 1:117:A:PRO:HB2 | 17       | 0.24          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2  | 2        | 0.24          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2  | 8        | 0.24          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2  | 10       | 0.24          |
| (1,288)  | 1:16:A:PHE:HA   | 1:64:A:LEU:HD23 | 13       | 0.24          |
| (1,201)  | 1:138:A:SER:H   | 1:137:A:ARG:HB2 | 19       | 0.24          |
| (1,110)  | 1:32:A:ILE:HG23 | 1:121:A:PRO:HG2 | 18       | 0.24          |
| (1,93)   | 1:4:A:ILE:HB    | 1:5:A:PRO:HD3   | 19       | 0.24          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2  | 17       | 0.24          |
| (1,33)   | 1:16:A:PHE:H    | 1:17:A:GLN:HB2  | 14       | 0.24          |
| (1,27)   | 1:60:A:GLN:HB3  | 1:54:A:LYS:HD2  | 7        | 0.24          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 2        | 0.23          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB   | 7        | 0.23          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 2        | 0.23          |
| (2,978)  | 1:65:A:PRO:CB   | 1:67:A:TRP:CB   | 14       | 0.23          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB  | 15       | 0.23          |
| (2,685)  | 1:103:A:SER:H   | 1:105:A:VAL:CB  | 8        | 0.23          |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB   | 1        | 0.23          |
| (2,560)  | 1:84:A:GLU:H    | 1:91:A:TRP:CB   | 7        | 0.23          |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB   | 15       | 0.23          |
| (2,444)  | 1:104:A:ASP:CB  | 1:36:A:VAL:CB   | 9        | 0.23          |
| (2,425)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 11       | 0.23          |
| (2,425)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 15       | 0.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,356)  | 1:31:A:PRO:CB    | 1:120:A:PHE:CB  | 2        | 0.23          |
| (2,324)  | 1:63:A:LEU:H     | 1:52:A:SER:CB   | 8        | 0.23          |
| (2,283)  | 1:81:A:SER:CB    | 1:84:A:GLU:CB   | 16       | 0.23          |
| (2,215)  | 1:29:A:GLY:H     | 1:124:A:THR:CB  | 12       | 0.23          |
| (2,130)  | 1:120:A:PHE:CB   | 1:30:A:VAL:CA   | 12       | 0.23          |
| (2,23)   | 1:115:A:ALA:H    | 1:114:A:GLU:CB  | 16       | 0.23          |
| (2,3)    | 1:46:A:TYR:CB    | 1:76:A:PRO:CB   | 2        | 0.23          |
| (2,3)    | 1:46:A:TYR:CB    | 1:76:A:PRO:CB   | 6        | 0.23          |
| (2,3)    | 1:46:A:TYR:CB    | 1:76:A:PRO:CB   | 16       | 0.23          |
| (1,1277) | 1:15:A:GLN:HA    | 1:64:A:LEU:HB3  | 10       | 0.23          |
| (1,1252) | 1:121:A:PRO:HA   | 1:32:A:ILE:HG12 | 6        | 0.23          |
| (1,1211) | 1:43:A:GLY:H     | 1:72:A:LEU:HB3  | 12       | 0.23          |
| (1,1210) | 1:43:A:GLY:H     | 1:92:A:VAL:HB   | 19       | 0.23          |
| (1,1167) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2  | 5        | 0.23          |
| (1,1167) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2  | 9        | 0.23          |
| (1,1142) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2  | 5        | 0.23          |
| (1,1142) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2  | 9        | 0.23          |
| (1,1120) | 1:130:A:TYR:H    | 1:13:A:ILE:HG23 | 19       | 0.23          |
| (1,1041) | 1:57:A:ASP:HA    | 1:58:A:GLY:H    | 11       | 0.23          |
| (1,970)  | 1:4:A:ILE:HB     | 1:6:A:HIS:HD2   | 7        | 0.23          |
| (1,970)  | 1:4:A:ILE:HB     | 1:6:A:HIS:HD2   | 14       | 0.23          |
| (1,851)  | 1:28:A:GLN:H     | 1:25:A:SER:HB3  | 18       | 0.23          |
| (1,839)  | 1:6:A:HIS:H      | 1:5:A:PRO:HG3   | 13       | 0.23          |
| (1,706)  | 1:61:A:LYS:H     | 1:60:A:GLN:HB2  | 16       | 0.23          |
| (1,605)  | 1:85:A:SER:HA    | 1:86:A:LEU:HB3  | 1        | 0.23          |
| (1,605)  | 1:85:A:SER:HA    | 1:86:A:LEU:HB3  | 10       | 0.23          |
| (1,605)  | 1:85:A:SER:HA    | 1:86:A:LEU:HB3  | 14       | 0.23          |
| (1,605)  | 1:85:A:SER:HA    | 1:86:A:LEU:HB3  | 16       | 0.23          |
| (1,471)  | 1:84:A:GLU:H     | 1:86:A:LEU:HD23 | 8        | 0.23          |
| (1,385)  | 1:118:A:THR:H    | 1:117:A:PRO:HB2 | 18       | 0.23          |
| (1,359)  | 1:72:A:LEU:H     | 1:71:A:TYR:HB2  | 17       | 0.23          |
| (1,324)  | 1:73:A:GLY:H     | 1:74:A:THR:HB   | 11       | 0.23          |
| (1,204)  | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3  | 4        | 0.23          |
| (1,109)  | 1:32:A:ILE:HG22  | 1:121:A:PRO:HG2 | 6        | 0.23          |
| (1,109)  | 1:32:A:ILE:HG21  | 1:121:A:PRO:HG2 | 6        | 0.23          |
| (1,109)  | 1:32:A:ILE:HG22  | 1:121:A:PRO:HG2 | 8        | 0.23          |
| (1,109)  | 1:32:A:ILE:HG21  | 1:121:A:PRO:HG2 | 8        | 0.23          |
| (1,93)   | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 4        | 0.23          |
| (1,93)   | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 6        | 0.23          |
| (1,93)   | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 13       | 0.23          |
| (1,78)   | 1:82:A:TYR:HB2   | 1:83:A:GLY:HA2  | 14       | 0.23          |
| (1,33)   | 1:16:A:PHE:H     | 1:17:A:GLN:HB2  | 17       | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB    | 17       | 0.22          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB   | 3        | 0.22          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB   | 4        | 0.22          |
| (2,1112) | 1:121:A:PRO:CA  | 1:32:A:ILE:CB    | 19       | 0.22          |
| (2,1087) | 1:137:A:ARG:H   | 1:11:A:SER:CB    | 10       | 0.22          |
| (2,1077) | 1:43:A:GLY:H    | 1:72:A:LEU:CB    | 19       | 0.22          |
| (2,1066) | 1:108:A:ARG:CA  | 1:9:A:TRP:CB     | 4        | 0.22          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB   | 19       | 0.22          |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB    | 11       | 0.22          |
| (2,749)  | 1:118:A:THR:CB  | 1:132:A:VAL:CB   | 17       | 0.22          |
| (2,645)  | 1:68:A:TYR:H    | 1:69:A:PHE:CB    | 9        | 0.22          |
| (2,521)  | 1:61:A:LYS:CB   | 1:63:A:LEU:CB    | 10       | 0.22          |
| (2,497)  | 1:54:A:LYS:CB   | 1:60:A:GLN:CB    | 17       | 0.22          |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H     | 18       | 0.22          |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB    | 12       | 0.22          |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB    | 13       | 0.22          |
| (2,444)  | 1:104:A:ASP:CB  | 1:36:A:VAL:CB    | 17       | 0.22          |
| (2,436)  | 1:33:A:ALA:CB   | 1:36:A:VAL:CB    | 19       | 0.22          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 8        | 0.22          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 10       | 0.22          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 17       | 0.22          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB   | 17       | 0.22          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 5        | 0.22          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 11       | 0.22          |
| (2,130)  | 1:120:A:PHE:CB  | 1:30:A:VAL:CA    | 5        | 0.22          |
| (2,81)   | 1:9:A:TRP:CB    | 1:71:A:TYR:CB    | 1        | 0.22          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H    | 7        | 0.22          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB    | 4        | 0.22          |
| (1,1140) | 1:50:A:ARG:HB3  | 1:66:A:ARG:HD2   | 13       | 0.22          |
| (1,1140) | 1:50:A:ARG:HB2  | 1:66:A:ARG:HD2   | 13       | 0.22          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H     | 2        | 0.22          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2   | 19       | 0.22          |
| (1,924)  | 1:71:A:TYR:HD2  | 1:105:A:VAL:HG23 | 18       | 0.22          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2  | 5        | 0.22          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2  | 11       | 0.22          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2  | 12       | 0.22          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2  | 14       | 0.22          |
| (1,839)  | 1:6:A:HIS:H     | 1:5:A:PRO:HG3    | 19       | 0.22          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA   | 1        | 0.22          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA   | 7        | 0.22          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA   | 10       | 0.22          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2   | 9        | 0.22          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,605) | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 3        | 0.22          |
| (1,605) | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 4        | 0.22          |
| (1,605) | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 8        | 0.22          |
| (1,605) | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 9        | 0.22          |
| (1,605) | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 12       | 0.22          |
| (1,605) | 1:85:A:SER:HA  | 1:86:A:LEU:HB3  | 18       | 0.22          |
| (1,509) | 1:44:A:TYR:H   | 1:72:A:LEU:H    | 18       | 0.22          |
| (1,471) | 1:84:A:GLU:H   | 1:86:A:LEU:HD23 | 9        | 0.22          |
| (1,364) | 1:82:A:TYR:H   | 1:83:A:GLY:H    | 5        | 0.22          |
| (1,364) | 1:82:A:TYR:H   | 1:83:A:GLY:H    | 11       | 0.22          |
| (1,333) | 1:81:A:SER:HA  | 1:84:A:GLU:HB3  | 6        | 0.22          |
| (1,333) | 1:81:A:SER:HA  | 1:84:A:GLU:HB3  | 13       | 0.22          |
| (1,201) | 1:138:A:SER:H  | 1:137:A:ARG:HB2 | 14       | 0.22          |
| (1,93)  | 1:4:A:ILE:HB   | 1:5:A:PRO:HD3   | 17       | 0.22          |
| (1,33)  | 1:16:A:PHE:H   | 1:17:A:GLN:HB2  | 18       | 0.22          |
| (1,26)  | 1:115:A:ALA:H  | 1:114:A:GLU:HG2 | 19       | 0.22          |
| (2,987) | 1:32:A:ILE:CB  | 1:121:A:PRO:CB  | 4        | 0.21          |
| (2,982) | 1:124:A:THR:H  | 1:125:A:ILE:CB  | 3        | 0.21          |
| (2,982) | 1:124:A:THR:H  | 1:125:A:ILE:CB  | 5        | 0.21          |
| (2,982) | 1:124:A:THR:H  | 1:125:A:ILE:CB  | 12       | 0.21          |
| (2,982) | 1:124:A:THR:H  | 1:125:A:ILE:CB  | 17       | 0.21          |
| (2,887) | 1:66:A:ARG:CB  | 1:68:A:TYR:CB   | 12       | 0.21          |
| (2,865) | 1:66:A:ARG:CB  | 1:68:A:TYR:CB   | 12       | 0.21          |
| (2,778) | 1:29:A:GLY:H   | 1:120:A:PHE:CB  | 8        | 0.21          |
| (2,749) | 1:118:A:THR:CB | 1:132:A:VAL:CB  | 3        | 0.21          |
| (2,749) | 1:118:A:THR:CB | 1:132:A:VAL:CB  | 5        | 0.21          |
| (2,697) | 1:119:A:ARG:H  | 1:31:A:PRO:CB   | 13       | 0.21          |
| (2,697) | 1:119:A:ARG:H  | 1:31:A:PRO:CB   | 18       | 0.21          |
| (2,654) | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 18       | 0.21          |
| (2,623) | 1:99:A:THR:CA  | 1:42:A:LYS:CB   | 19       | 0.21          |
| (2,571) | 1:89:A:VAL:CB  | 1:45:A:TRP:CB   | 7        | 0.21          |
| (2,564) | 1:127:A:PRO:CB | 1:23:A:LYS:CB   | 4        | 0.21          |
| (2,564) | 1:127:A:PRO:CB | 1:23:A:LYS:CB   | 15       | 0.21          |
| (2,469) | 1:44:A:TYR:H   | 1:72:A:LEU:H    | 10       | 0.21          |
| (2,466) | 1:41:A:ALA:CA  | 1:30:A:VAL:CB   | 3        | 0.21          |
| (2,466) | 1:41:A:ALA:CA  | 1:30:A:VAL:CB   | 9        | 0.21          |
| (2,443) | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 4        | 0.21          |
| (2,443) | 1:36:A:VAL:CB  | 1:37:A:PRO:CB   | 16       | 0.21          |
| (2,436) | 1:33:A:ALA:CB  | 1:36:A:VAL:CB   | 16       | 0.21          |
| (2,431) | 1:120:A:PHE:H  | 1:32:A:ILE:CB   | 4        | 0.21          |
| (2,431) | 1:120:A:PHE:H  | 1:32:A:ILE:CB   | 16       | 0.21          |
| (2,324) | 1:63:A:LEU:H   | 1:52:A:SER:CB   | 18       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,261)  | 1:108:A:ARG:H   | 1:107:A:SER:H   | 13       | 0.21          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H   | 17       | 0.21          |
| (2,33)   | 1:104:A:ASP:H   | 1:105:A:VAL:CB  | 13       | 0.21          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 11       | 0.21          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 9        | 0.21          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 6        | 0.21          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 10       | 0.21          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 12       | 0.21          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 18       | 0.21          |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 1        | 0.21          |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 7        | 0.21          |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 1        | 0.21          |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 7        | 0.21          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 3        | 0.21          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 12       | 0.21          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 13       | 0.21          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 16       | 0.21          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 19       | 0.21          |
| (1,1017) | 1:29:A:GLY:H    | 1:28:A:GLN:HB3  | 17       | 0.21          |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD1 | 14       | 0.21          |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD2 | 14       | 0.21          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 2        | 0.21          |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 13       | 0.21          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 4        | 0.21          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 9        | 0.21          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 2        | 0.21          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 14       | 0.21          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 16       | 0.21          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 18       | 0.21          |
| (1,626)  | 1:89:A:VAL:HG13 | 1:86:A:LEU:HD21 | 15       | 0.21          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3  | 2        | 0.21          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3  | 17       | 0.21          |
| (1,595)  | 1:115:A:ALA:HA  | 1:114:A:GLU:HB2 | 19       | 0.21          |
| (1,537)  | 1:54:A:LYS:HB2  | 1:60:A:GLN:HB3  | 12       | 0.21          |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 2        | 0.21          |
| (1,509)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 10       | 0.21          |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23 | 3        | 0.21          |
| (1,343)  | 1:97:A:ALA:H    | 1:39:A:SER:HA   | 9        | 0.21          |
| (1,343)  | 1:97:A:ALA:H    | 1:39:A:SER:HA   | 12       | 0.21          |
| (1,302)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:H    | 11       | 0.21          |
| (1,292)  | 1:17:A:GLN:H    | 1:16:A:PHE:HB3  | 8        | 0.21          |
| (1,284)  | 1:108:A:ARG:H   | 1:107:A:SER:H   | 13       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,259)  | 1:10:A:PHE:HA   | 1:8:A:SER:HA    | 10       | 0.21          |
| (1,221)  | 1:111:A:THR:H   | 1:110:A:PRO:HG3 | 13       | 0.21          |
| (1,201)  | 1:138:A:SER:H   | 1:137:A:ARG:HB2 | 2        | 0.21          |
| (1,138)  | 1:138:A:SER:H   | 1:137:A:ARG:HA  | 18       | 0.21          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG22  | 1        | 0.21          |
| (1,124)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG21  | 1        | 0.21          |
| (2,1087) | 1:137:A:ARG:H   | 1:11:A:SER:CB   | 5        | 0.2           |
| (2,1077) | 1:43:A:GLY:H    | 1:72:A:LEU:CB   | 4        | 0.2           |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB   | 2        | 0.2           |
| (2,987)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 17       | 0.2           |
| (2,986)  | 1:102:A:PRO:CB  | 1:72:A:LEU:CB   | 2        | 0.2           |
| (2,984)  | 1:119:A:ARG:CB  | 1:117:A:PRO:CB  | 15       | 0.2           |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 12       | 0.2           |
| (2,887)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB   | 15       | 0.2           |
| (2,865)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB   | 15       | 0.2           |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB   | 12       | 0.2           |
| (2,654)  | 1:71:A:TYR:CB   | 1:105:A:VAL:CB  | 9        | 0.2           |
| (2,623)  | 1:99:A:THR:CA   | 1:42:A:LYS:CB   | 12       | 0.2           |
| (2,571)  | 1:89:A:VAL:CB   | 1:45:A:TRP:CB   | 19       | 0.2           |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 4        | 0.2           |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 4        | 0.2           |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 9        | 0.2           |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 9        | 0.2           |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 14       | 0.2           |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 14       | 0.2           |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 14       | 0.2           |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB   | 2        | 0.2           |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB   | 7        | 0.2           |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 4        | 0.2           |
| (2,445)  | 1:40:A:GLU:CB   | 1:36:A:VAL:CB   | 4        | 0.2           |
| (2,443)  | 1:36:A:VAL:CB   | 1:37:A:PRO:CB   | 19       | 0.2           |
| (2,425)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 4        | 0.2           |
| (2,425)  | 1:132:A:VAL:H   | 1:126:A:LEU:CB  | 5        | 0.2           |
| (2,362)  | 1:104:A:ASP:H   | 1:40:A:GLU:CB   | 18       | 0.2           |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 14       | 0.2           |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB   | 7        | 0.2           |
| (2,261)  | 1:108:A:ARG:H   | 1:107:A:SER:H   | 19       | 0.2           |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 12       | 0.2           |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H   | 12       | 0.2           |
| (2,68)   | 1:86:A:LEU:H    | 1:45:A:TRP:CB   | 11       | 0.2           |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 4        | 0.2           |
| (1,1274) | 1:134:A:GLY:HA2 | 1:117:A:PRO:HD3 | 1        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 2        | 0.2           |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 4        | 0.2           |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 16       | 0.2           |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 17       | 0.2           |
| (1,1096) | 1:119:A:ARG:HG3 | 1:117:A:PRO:HG3 | 8        | 0.2           |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 8        | 0.2           |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 9        | 0.2           |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 10       | 0.2           |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 15       | 0.2           |
| (1,1011) | 1:42:A:LYS:HG2  | 1:72:A:LEU:HG   | 8        | 0.2           |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD1 | 3        | 0.2           |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD2 | 3        | 0.2           |
| (1,847)  | 1:122:A:PRO:HD2 | 1:121:A:PRO:HB2 | 1        | 0.2           |
| (1,840)  | 1:120:A:PHE:HA  | 1:32:A:ILE:HG12 | 8        | 0.2           |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 12       | 0.2           |
| (1,745)  | 1:91:A:TRP:H    | 1:90:A:PHE:HB3  | 7        | 0.2           |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 12       | 0.2           |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 5        | 0.2           |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 8        | 0.2           |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 12       | 0.2           |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 19       | 0.2           |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 8        | 0.2           |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 9        | 0.2           |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 10       | 0.2           |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 17       | 0.2           |
| (1,653)  | 1:16:A:PHE:H    | 1:64:A:LEU:HD21 | 15       | 0.2           |
| (1,648)  | 1:15:A:GLN:H    | 1:13:A:ILE:HG23 | 8        | 0.2           |
| (1,595)  | 1:115:A:ALA:HA  | 1:114:A:GLU:HB2 | 13       | 0.2           |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 12       | 0.2           |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 13       | 0.2           |
| (1,517)  | 1:43:A:GLY:HA2  | 1:70:A:TYR:HA   | 16       | 0.2           |
| (1,509)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 14       | 0.2           |
| (1,485)  | 1:40:A:GLU:HB3  | 1:36:A:VAL:HG23 | 19       | 0.2           |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1  | 5        | 0.2           |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2  | 5        | 0.2           |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2  | 3        | 0.2           |
| (1,284)  | 1:108:A:ARG:H   | 1:107:A:SER:H   | 19       | 0.2           |
| (1,221)  | 1:111:A:THR:H   | 1:110:A:PRO:HG3 | 12       | 0.2           |
| (1,109)  | 1:32:A:ILE:HG22 | 1:121:A:PRO:HG2 | 9        | 0.2           |
| (1,109)  | 1:32:A:ILE:HG21 | 1:121:A:PRO:HG2 | 9        | 0.2           |
| (1,78)   | 1:82:A:TYR:HB2  | 1:83:A:GLY:HA2  | 15       | 0.2           |
| (2,1112) | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 8        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1099) | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 5        | 0.19          |
| (2,982)  | 1:124:A:THR:H   | 1:125:A:ILE:CB  | 4        | 0.19          |
| (2,982)  | 1:124:A:THR:H   | 1:125:A:ILE:CB  | 8        | 0.19          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB  | 3        | 0.19          |
| (2,885)  | 1:32:A:ILE:CB   | 1:120:A:PHE:CB  | 17       | 0.19          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 6        | 0.19          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 6        | 0.19          |
| (2,778)  | 1:29:A:GLY:H    | 1:120:A:PHE:CB  | 7        | 0.19          |
| (2,606)  | 1:32:A:ILE:CB   | 1:34:A:PHE:H    | 15       | 0.19          |
| (2,536)  | 1:79:A:ASN:CA   | 1:72:A:LEU:CB   | 14       | 0.19          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 1        | 0.19          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 1        | 0.19          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 5        | 0.19          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 11       | 0.19          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 17       | 0.19          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 1        | 0.19          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 17       | 0.19          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB   | 6        | 0.19          |
| (2,263)  | 1:16:A:PHE:CA   | 1:64:A:LEU:CB   | 16       | 0.19          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H   | 4        | 0.19          |
| (2,23)   | 1:115:A:ALA:H   | 1:114:A:GLU:CB  | 17       | 0.19          |
| (1,1277) | 1:15:A:GLN:HA   | 1:64:A:LEU:HB3  | 15       | 0.19          |
| (1,1272) | 1:129:A:GLY:HA3 | 1:17:A:GLN:HB2  | 9        | 0.19          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3  | 16       | 0.19          |
| (1,1211) | 1:43:A:GLY:H    | 1:72:A:LEU:HB3  | 11       | 0.19          |
| (1,1211) | 1:43:A:GLY:H    | 1:72:A:LEU:HB3  | 13       | 0.19          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 1        | 0.19          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB   | 5        | 0.19          |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 6        | 0.19          |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2  | 6        | 0.19          |
| (1,736)  | 1:113:A:GLN:HA  | 1:108:A:ARG:HD2 | 15       | 0.19          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA  | 9        | 0.19          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 3        | 0.19          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 13       | 0.19          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 15       | 0.19          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 16       | 0.19          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 19       | 0.19          |
| (1,485)  | 1:40:A:GLU:HB3  | 1:36:A:VAL:HG23 | 7        | 0.19          |
| (1,402)  | 1:32:A:ILE:HD12 | 1:121:A:PRO:HG2 | 3        | 0.19          |
| (1,402)  | 1:32:A:ILE:HD11 | 1:121:A:PRO:HG2 | 3        | 0.19          |
| (1,402)  | 1:32:A:ILE:HD13 | 1:121:A:PRO:HG2 | 3        | 0.19          |
| (1,385)  | 1:118:A:THR:H   | 1:117:A:PRO:HB2 | 13       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,364)  | 1:82:A:TYR:H   | 1:83:A:GLY:H    | 1        | 0.19          |
| (1,364)  | 1:82:A:TYR:H   | 1:83:A:GLY:H    | 17       | 0.19          |
| (1,334)  | 1:138:A:SER:H  | 1:134:A:GLY:HA3 | 3        | 0.19          |
| (1,324)  | 1:73:A:GLY:H   | 1:74:A:THR:HB   | 3        | 0.19          |
| (1,302)  | 1:43:A:GLY:HA3 | 1:72:A:LEU:H    | 10       | 0.19          |
| (1,221)  | 1:111:A:THR:H  | 1:110:A:PRO:HG3 | 9        | 0.19          |
| (1,168)  | 1:7:A:TYR:HD1  | 1:110:A:PRO:HG3 | 12       | 0.19          |
| (1,168)  | 1:7:A:TYR:HD2  | 1:110:A:PRO:HG3 | 12       | 0.19          |
| (1,138)  | 1:138:A:SER:H  | 1:137:A:ARG:HA  | 3        | 0.19          |
| (1,83)   | 1:46:A:TYR:HD1 | 1:76:A:PRO:HD3  | 6        | 0.19          |
| (1,83)   | 1:46:A:TYR:HD2 | 1:76:A:PRO:HD3  | 6        | 0.19          |
| (1,47)   | 1:25:A:SER:HA  | 1:28:A:GLN:HB3  | 16       | 0.19          |
| (2,1149) | 1:18:A:LYS:CB  | 1:64:A:LEU:CB   | 18       | 0.18          |
| (2,1148) | 1:64:A:LEU:CB  | 1:18:A:LYS:CB   | 18       | 0.18          |
| (2,1116) | 1:82:A:TYR:CA  | 1:72:A:LEU:CB   | 11       | 0.18          |
| (2,986)  | 1:102:A:PRO:CB | 1:72:A:LEU:CB   | 6        | 0.18          |
| (2,982)  | 1:124:A:THR:H  | 1:125:A:ILE:CB  | 2        | 0.18          |
| (2,926)  | 1:101:A:THR:CB | 1:100:A:SER:CB  | 1        | 0.18          |
| (2,887)  | 1:66:A:ARG:CB  | 1:68:A:TYR:CB   | 16       | 0.18          |
| (2,865)  | 1:66:A:ARG:CB  | 1:68:A:TYR:CB   | 16       | 0.18          |
| (2,854)  | 1:14:A:THR:CA  | 1:66:A:ARG:CB   | 15       | 0.18          |
| (2,699)  | 1:111:A:THR:CB | 1:110:A:PRO:CB  | 17       | 0.18          |
| (2,685)  | 1:103:A:SER:H  | 1:105:A:VAL:CB  | 14       | 0.18          |
| (2,657)  | 1:72:A:LEU:H   | 1:42:A:LYS:CB   | 8        | 0.18          |
| (2,654)  | 1:71:A:TYR:CB  | 1:105:A:VAL:CB  | 15       | 0.18          |
| (2,645)  | 1:68:A:TYR:H   | 1:69:A:PHE:CB   | 11       | 0.18          |
| (2,536)  | 1:79:A:ASN:CA  | 1:72:A:LEU:CB   | 9        | 0.18          |
| (2,526)  | 1:39:A:SER:H   | 1:96:A:GLN:CB   | 2        | 0.18          |
| (2,526)  | 1:39:A:SER:H   | 1:96:A:GLN:CB   | 2        | 0.18          |
| (2,471)  | 1:41:A:ALA:CB  | 1:94:A:ASN:CB   | 15       | 0.18          |
| (2,440)  | 1:91:A:TRP:H   | 1:89:A:VAL:CB   | 7        | 0.18          |
| (2,396)  | 1:15:A:GLN:H   | 1:64:A:LEU:CB   | 12       | 0.18          |
| (2,396)  | 1:15:A:GLN:H   | 1:64:A:LEU:CB   | 17       | 0.18          |
| (2,339)  | 1:82:A:TYR:H   | 1:83:A:GLY:H    | 8        | 0.18          |
| (2,338)  | 1:66:A:ARG:H   | 1:48:A:HIS:CB   | 18       | 0.18          |
| (2,261)  | 1:108:A:ARG:H  | 1:107:A:SER:H   | 15       | 0.18          |
| (2,241)  | 1:101:A:THR:CB | 1:100:A:SER:CB  | 1        | 0.18          |
| (2,177)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 17       | 0.18          |
| (2,177)  | 1:116:A:ILE:CA | 1:117:A:PRO:CB  | 19       | 0.18          |
| (2,164)  | 1:69:A:PHE:CB  | 1:10:A:PHE:CB   | 3        | 0.18          |
| (2,156)  | 1:4:A:ILE:CB   | 1:6:A:HIS:CB    | 5        | 0.18          |
| (2,156)  | 1:4:A:ILE:CB   | 1:6:A:HIS:CB    | 15       | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB   | 5        | 0.18          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H    | 3        | 0.18          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H    | 9        | 0.18          |
| (2,33)   | 1:104:A:ASP:H   | 1:105:A:VAL:CB   | 2        | 0.18          |
| (2,33)   | 1:104:A:ASP:H   | 1:105:A:VAL:CB   | 17       | 0.18          |
| (1,1266) | 1:51:A:ARG:HB2  | 1:63:A:LEU:HD21  | 3        | 0.18          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3   | 1        | 0.18          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3   | 10       | 0.18          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB    | 3        | 0.18          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB    | 8        | 0.18          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB    | 9        | 0.18          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB    | 13       | 0.18          |
| (1,1173) | 1:51:A:ARG:HB2  | 1:63:A:LEU:HD21  | 3        | 0.18          |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 15       | 0.18          |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 15       | 0.18          |
| (1,1120) | 1:130:A:TYR:H   | 1:13:A:ILE:HG23  | 1        | 0.18          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H     | 17       | 0.18          |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD1  | 11       | 0.18          |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD2  | 11       | 0.18          |
| (1,950)  | 1:8:A:SER:HB2   | 1:7:A:TYR:HA     | 7        | 0.18          |
| (1,937)  | 1:69:A:PHE:HB2  | 1:31:A:PRO:HG2   | 7        | 0.18          |
| (1,927)  | 1:71:A:TYR:HE2  | 1:105:A:VAL:HG23 | 12       | 0.18          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2   | 16       | 0.18          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3   | 3        | 0.18          |
| (1,745)  | 1:91:A:TRP:H    | 1:90:A:PHE:HB3   | 9        | 0.18          |
| (1,725)  | 1:72:A:LEU:H    | 1:102:A:PRO:HA   | 18       | 0.18          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2   | 4        | 0.18          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2   | 14       | 0.18          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3   | 2        | 0.18          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3   | 11       | 0.18          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3   | 12       | 0.18          |
| (1,605)  | 1:85:A:SER:HA   | 1:86:A:LEU:HB3   | 7        | 0.18          |
| (1,416)  | 1:97:A:ALA:H    | 1:96:A:GLN:HB3   | 3        | 0.18          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1   | 2        | 0.18          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2   | 2        | 0.18          |
| (1,380)  | 1:31:A:PRO:HA   | 1:32:A:ILE:HG12  | 7        | 0.18          |
| (1,365)  | 1:29:A:GLY:HA3  | 1:30:A:VAL:H     | 12       | 0.18          |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H     | 8        | 0.18          |
| (1,355)  | 1:82:A:TYR:H    | 1:81:A:SER:HB3   | 19       | 0.18          |
| (1,349)  | 1:63:A:LEU:H    | 1:52:A:SER:HB2   | 18       | 0.18          |
| (1,324)  | 1:73:A:GLY:H    | 1:74:A:THR:HB    | 7        | 0.18          |
| (1,302)  | 1:43:A:GLY:HA3  | 1:72:A:LEU:H     | 4        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,284)  | 1:108:A:ARG:H   | 1:107:A:SER:H   | 15       | 0.18          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2  | 12       | 0.18          |
| (1,109)  | 1:32:A:ILE:HG22 | 1:121:A:PRO:HG2 | 18       | 0.18          |
| (1,109)  | 1:32:A:ILE:HG21 | 1:121:A:PRO:HG2 | 18       | 0.18          |
| (1,95)   | 1:34:A:PHE:HD2  | 1:71:A:TYR:HE1  | 12       | 0.18          |
| (1,93)   | 1:4:A:ILE:HB    | 1:5:A:PRO:HD3   | 10       | 0.18          |
| (1,83)   | 1:46:A:TYR:HD1  | 1:76:A:PRO:HD3  | 13       | 0.18          |
| (1,83)   | 1:46:A:TYR:HD2  | 1:76:A:PRO:HD3  | 13       | 0.18          |
| (1,33)   | 1:16:A:PHE:H    | 1:17:A:GLN:HB2  | 5        | 0.18          |
| (1,26)   | 1:115:A:ALA:H   | 1:114:A:GLU:HG2 | 2        | 0.18          |
| (2,1126) | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 11       | 0.17          |
| (2,1112) | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 9        | 0.17          |
| (2,1112) | 1:121:A:PRO:CA  | 1:32:A:ILE:CB   | 18       | 0.17          |
| (2,982)  | 1:124:A:THR:H   | 1:125:A:ILE:CB  | 10       | 0.17          |
| (2,956)  | 1:9:A:TRP:CB    | 1:107:A:SER:CB  | 14       | 0.17          |
| (2,887)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB   | 10       | 0.17          |
| (2,865)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB   | 10       | 0.17          |
| (2,749)  | 1:118:A:THR:CB  | 1:132:A:VAL:CB  | 15       | 0.17          |
| (2,718)  | 1:42:A:LYS:H    | 1:40:A:GLU:CB   | 10       | 0.17          |
| (2,718)  | 1:42:A:LYS:H    | 1:40:A:GLU:CB   | 13       | 0.17          |
| (2,685)  | 1:103:A:SER:H   | 1:105:A:VAL:CB  | 19       | 0.17          |
| (2,635)  | 1:59:A:GLN:H    | 1:54:A:LYS:CB   | 9        | 0.17          |
| (2,595)  | 1:17:A:GLN:H    | 1:64:A:LEU:CB   | 12       | 0.17          |
| (2,571)  | 1:89:A:VAL:CB   | 1:45:A:TRP:CB   | 13       | 0.17          |
| (2,537)  | 1:124:A:THR:H   | 1:28:A:GLN:CB   | 7        | 0.17          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 5        | 0.17          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 5        | 0.17          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 9        | 0.17          |
| (2,426)  | 1:40:A:GLU:H    | 1:36:A:VAL:CB   | 4        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 1        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 2        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 3        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 4        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 6        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 8        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 9        | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 11       | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 12       | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 13       | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 14       | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 16       | 0.17          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 18       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 16       | 0.17          |
| (2,30)   | 1:16:A:PHE:H    | 1:17:A:GLN:CB   | 3        | 0.17          |
| (2,23)   | 1:115:A:ALA:H   | 1:114:A:GLU:CB  | 13       | 0.17          |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 18       | 0.17          |
| (1,1261) | 1:7:A:TYR:H     | 1:6:A:HIS:HB2   | 15       | 0.17          |
| (1,1252) | 1:121:A:PRO:HA  | 1:32:A:ILE:HG12 | 9        | 0.17          |
| (1,1041) | 1:57:A:ASP:HA   | 1:58:A:GLY:H    | 18       | 0.17          |
| (1,1011) | 1:42:A:LYS:HG2  | 1:72:A:LEU:HG   | 14       | 0.17          |
| (1,1005) | 1:135:A:SER:HA  | 1:117:A:PRO:HD2 | 8        | 0.17          |
| (1,874)  | 1:126:A:LEU:HB2 | 1:127:A:PRO:HD3 | 16       | 0.17          |
| (1,790)  | 1:42:A:LYS:H    | 1:40:A:GLU:HB2  | 4        | 0.17          |
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 2        | 0.17          |
| (1,745)  | 1:91:A:TRP:H    | 1:90:A:PHE:HB3  | 16       | 0.17          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2  | 2        | 0.17          |
| (1,607)  | 1:127:A:PRO:HG2 | 1:23:A:LYS:HG2  | 14       | 0.17          |
| (1,508)  | 1:41:A:ALA:HA   | 1:71:A:TYR:HE2  | 16       | 0.17          |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23 | 1        | 0.17          |
| (1,402)  | 1:32:A:ILE:HD12 | 1:121:A:PRO:HG2 | 1        | 0.17          |
| (1,402)  | 1:32:A:ILE:HD11 | 1:121:A:PRO:HG2 | 1        | 0.17          |
| (1,402)  | 1:32:A:ILE:HD13 | 1:121:A:PRO:HG2 | 1        | 0.17          |
| (1,385)  | 1:118:A:THR:H   | 1:117:A:PRO:HB2 | 19       | 0.17          |
| (1,343)  | 1:97:A:ALA:H    | 1:39:A:SER:HA   | 10       | 0.17          |
| (1,221)  | 1:111:A:THR:H   | 1:110:A:PRO:HG3 | 15       | 0.17          |
| (1,173)  | 1:36:A:VAL:H    | 1:35:A:GLY:HA2  | 8        | 0.17          |
| (1,152)  | 1:114:A:GLU:HA  | 1:115:A:ALA:H   | 1        | 0.17          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3  | 9        | 0.17          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3  | 15       | 0.17          |
| (2,1200) | 1:130:A:TYR:CB  | 1:126:A:LEU:CB  | 5        | 0.16          |
| (2,1124) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 10       | 0.16          |
| (2,1077) | 1:43:A:GLY:H    | 1:72:A:LEU:CB   | 10       | 0.16          |
| (2,1044) | 1:51:A:ARG:CB   | 1:63:A:LEU:CB   | 10       | 0.16          |
| (2,986)  | 1:102:A:PRO:CB  | 1:72:A:LEU:CB   | 7        | 0.16          |
| (2,986)  | 1:102:A:PRO:CB  | 1:72:A:LEU:CB   | 15       | 0.16          |
| (2,986)  | 1:102:A:PRO:CB  | 1:72:A:LEU:CB   | 17       | 0.16          |
| (2,982)  | 1:124:A:THR:H   | 1:125:A:ILE:CB  | 16       | 0.16          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB  | 17       | 0.16          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 10       | 0.16          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 11       | 0.16          |
| (2,926)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 19       | 0.16          |
| (2,885)  | 1:32:A:ILE:CB   | 1:120:A:PHE:CB  | 16       | 0.16          |
| (2,749)  | 1:118:A:THR:CB  | 1:132:A:VAL:CB  | 9        | 0.16          |
| (2,699)  | 1:111:A:THR:CB  | 1:110:A:PRO:CB  | 2        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,699)  | 1:111:A:THR:CB  | 1:110:A:PRO:CB  | 13       | 0.16          |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB   | 3        | 0.16          |
| (2,571)  | 1:89:A:VAL:CB   | 1:45:A:TRP:CB   | 8        | 0.16          |
| (2,564)  | 1:127:A:PRO:CB  | 1:23:A:LYS:CB   | 11       | 0.16          |
| (2,560)  | 1:84:A:GLU:H    | 1:91:A:TRP:CB   | 6        | 0.16          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 8        | 0.16          |
| (2,526)  | 1:39:A:SER:H    | 1:96:A:GLN:CB   | 8        | 0.16          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 2        | 0.16          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 8        | 0.16          |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 13       | 0.16          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB   | 9        | 0.16          |
| (2,369)  | 1:96:A:GLN:CB   | 1:38:A:PRO:CB   | 3        | 0.16          |
| (2,356)  | 1:31:A:PRO:CB   | 1:120:A:PHE:CB  | 13       | 0.16          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 10       | 0.16          |
| (2,339)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 18       | 0.16          |
| (2,263)  | 1:16:A:PHE:CA   | 1:64:A:LEU:CB   | 13       | 0.16          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 10       | 0.16          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 11       | 0.16          |
| (2,241)  | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 19       | 0.16          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 5        | 0.16          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 7        | 0.16          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 10       | 0.16          |
| (2,177)  | 1:116:A:ILE:CA  | 1:117:A:PRO:CB  | 15       | 0.16          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 2        | 0.16          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 6        | 0.16          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 7        | 0.16          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 9        | 0.16          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 14       | 0.16          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB  | 18       | 0.16          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H   | 16       | 0.16          |
| (2,33)   | 1:104:A:ASP:H   | 1:105:A:VAL:CB  | 8        | 0.16          |
| (2,3)    | 1:46:A:TYR:CB   | 1:76:A:PRO:CB   | 19       | 0.16          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2  | 19       | 0.16          |
| (1,1261) | 1:7:A:TYR:H     | 1:6:A:HIS:HB2   | 10       | 0.16          |
| (1,1168) | 1:62:A:GLN:HA   | 1:52:A:SER:HB2  | 11       | 0.16          |
| (1,1156) | 1:63:A:LEU:HA   | 1:62:A:GLN:HB2  | 4        | 0.16          |
| (1,1156) | 1:63:A:LEU:HA   | 1:62:A:GLN:HB2  | 8        | 0.16          |
| (1,1143) | 1:62:A:GLN:HA   | 1:52:A:SER:HB2  | 11       | 0.16          |
| (1,1103) | 1:55:A:THR:H    | 1:54:A:LYS:HD3  | 1        | 0.16          |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD1 | 13       | 0.16          |
| (1,987)  | 1:32:A:ILE:HG12 | 1:120:A:PHE:HD2 | 13       | 0.16          |
| (1,950)  | 1:8:A:SER:HB2   | 1:7:A:TYR:HA    | 2        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,771)  | 1:83:A:GLY:H    | 1:84:A:GLU:HB3  | 7        | 0.16          |
| (1,745)  | 1:91:A:TRP:H    | 1:90:A:PHE:HB3  | 3        | 0.16          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3  | 5        | 0.16          |
| (1,631)  | 1:89:A:VAL:HG23 | 1:86:A:LEU:HB3  | 7        | 0.16          |
| (1,599)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD22 | 4        | 0.16          |
| (1,599)  | 1:84:A:GLU:HB2  | 1:86:A:LEU:HD22 | 8        | 0.16          |
| (1,509)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 13       | 0.16          |
| (1,508)  | 1:41:A:ALA:HA   | 1:71:A:TYR:HE2  | 12       | 0.16          |
| (1,459)  | 1:24:A:PHE:H    | 1:23:A:LYS:HG3  | 14       | 0.16          |
| (1,402)  | 1:32:A:ILE:HD12 | 1:121:A:PRO:HG2 | 14       | 0.16          |
| (1,402)  | 1:32:A:ILE:HD11 | 1:121:A:PRO:HG2 | 14       | 0.16          |
| (1,402)  | 1:32:A:ILE:HD13 | 1:121:A:PRO:HG2 | 14       | 0.16          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1  | 7        | 0.16          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2  | 7        | 0.16          |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 10       | 0.16          |
| (1,364)  | 1:82:A:TYR:H    | 1:83:A:GLY:H    | 18       | 0.16          |
| (1,359)  | 1:72:A:LEU:H    | 1:71:A:TYR:HB2  | 19       | 0.16          |
| (1,351)  | 1:130:A:TYR:H   | 1:129:A:GLY:HA2 | 4        | 0.16          |
| (1,343)  | 1:97:A:ALA:H    | 1:39:A:SER:HA   | 5        | 0.16          |
| (1,281)  | 1:109:A:ASP:H   | 1:108:A:ARG:HB3 | 9        | 0.16          |
| (1,221)  | 1:111:A:THR:H   | 1:110:A:PRO:HG3 | 17       | 0.16          |
| (1,152)  | 1:114:A:GLU:HA  | 1:115:A:ALA:H   | 6        | 0.16          |
| (1,125)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG23  | 9        | 0.16          |
| (1,125)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG23  | 17       | 0.16          |
| (1,93)   | 1:4:A:ILE:HB    | 1:5:A:PRO:HD3   | 1        | 0.16          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3  | 11       | 0.16          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 18       | 0.16          |
| (1,42)   | 1:63:A:LEU:HA   | 1:52:A:SER:HB2  | 19       | 0.16          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB   | 9        | 0.15          |
| (2,1126) | 1:20:A:ARG:CB   | 1:128:A:GLN:CB  | 14       | 0.15          |
| (2,1066) | 1:108:A:ARG:CA  | 1:9:A:TRP:CB    | 2        | 0.15          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB   | 12       | 0.15          |
| (2,987)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB  | 16       | 0.15          |
| (2,986)  | 1:102:A:PRO:CB  | 1:72:A:LEU:CB   | 9        | 0.15          |
| (2,982)  | 1:124:A:THR:H   | 1:125:A:ILE:CB  | 11       | 0.15          |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB  | 18       | 0.15          |
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 13       | 0.15          |
| (2,868)  | 1:4:A:ILE:CB    | 1:6:A:HIS:CB    | 9        | 0.15          |
| (2,856)  | 1:6:A:HIS:CB    | 1:4:A:ILE:CB    | 9        | 0.15          |
| (2,854)  | 1:14:A:THR:CA   | 1:66:A:ARG:CB   | 2        | 0.15          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 10       | 0.15          |
| (2,802)  | 1:132:A:VAL:CB  | 1:126:A:LEU:CB  | 10       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,705)  | 1:125:A:ILE:H   | 1:25:A:SER:CB    | 17       | 0.15          |
| (2,697)  | 1:119:A:ARG:H   | 1:31:A:PRO:CB    | 6        | 0.15          |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB    | 4        | 0.15          |
| (2,643)  | 1:68:A:TYR:H    | 1:48:A:HIS:H     | 17       | 0.15          |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB    | 5        | 0.15          |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB    | 17       | 0.15          |
| (2,440)  | 1:91:A:TRP:H    | 1:89:A:VAL:CB    | 19       | 0.15          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 13       | 0.15          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 14       | 0.15          |
| (2,362)  | 1:104:A:ASP:H   | 1:40:A:GLU:CB    | 5        | 0.15          |
| (2,362)  | 1:104:A:ASP:H   | 1:40:A:GLU:CB    | 7        | 0.15          |
| (2,324)  | 1:63:A:LEU:H    | 1:52:A:SER:CB    | 16       | 0.15          |
| (2,217)  | 1:89:A:VAL:CB   | 1:45:A:TRP:CB    | 16       | 0.15          |
| (2,188)  | 1:125:A:ILE:CB  | 1:23:A:LYS:CB    | 5        | 0.15          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB   | 15       | 0.15          |
| (2,79)   | 1:101:A:THR:CB  | 1:100:A:SER:CB   | 17       | 0.15          |
| (2,74)   | 1:13:A:ILE:CA   | 1:133:A:GLU:H    | 19       | 0.15          |
| (2,30)   | 1:16:A:PHE:H    | 1:17:A:GLN:CB    | 1        | 0.15          |
| (2,24)   | 1:60:A:GLN:CB   | 1:54:A:LYS:CB    | 17       | 0.15          |
| (2,9)    | 1:4:A:ILE:CB    | 1:6:A:HIS:CB     | 19       | 0.15          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2   | 3        | 0.15          |
| (1,1273) | 1:129:A:GLY:HA3 | 1:20:A:ARG:HG2   | 16       | 0.15          |
| (1,1272) | 1:129:A:GLY:HA3 | 1:17:A:GLN:HB2   | 19       | 0.15          |
| (1,1256) | 1:27:A:GLY:H    | 1:28:A:GLN:HB3   | 15       | 0.15          |
| (1,1252) | 1:121:A:PRO:HA  | 1:32:A:ILE:HG12  | 8        | 0.15          |
| (1,1211) | 1:43:A:GLY:H    | 1:72:A:LEU:HB3   | 1        | 0.15          |
| (1,1210) | 1:43:A:GLY:H    | 1:92:A:VAL:HB    | 7        | 0.15          |
| (1,1167) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 16       | 0.15          |
| (1,1156) | 1:63:A:LEU:HA   | 1:62:A:GLN:HB2   | 3        | 0.15          |
| (1,1142) | 1:51:A:ARG:HA   | 1:52:A:SER:HB2   | 16       | 0.15          |
| (1,1128) | 1:73:A:GLY:HA3  | 1:102:A:PRO:HG2  | 15       | 0.15          |
| (1,1012) | 1:64:A:LEU:H    | 1:63:A:LEU:HB3   | 2        | 0.15          |
| (1,1011) | 1:42:A:LYS:HG2  | 1:72:A:LEU:HG    | 5        | 0.15          |
| (1,950)  | 1:8:A:SER:HB2   | 1:7:A:TYR:HA     | 3        | 0.15          |
| (1,924)  | 1:71:A:TYR:HD2  | 1:105:A:VAL:HG23 | 8        | 0.15          |
| (1,888)  | 1:20:A:ARG:HD2  | 1:128:A:GLN:HG3  | 3        | 0.15          |
| (1,768)  | 1:119:A:ARG:H   | 1:31:A:PRO:HB3   | 6        | 0.15          |
| (1,712)  | 1:68:A:TYR:H    | 1:48:A:HIS:H     | 17       | 0.15          |
| (1,706)  | 1:61:A:LYS:H    | 1:60:A:GLN:HB2   | 7        | 0.15          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3   | 7        | 0.15          |
| (1,702)  | 1:58:A:GLY:H    | 1:57:A:ASP:HB3   | 14       | 0.15          |
| (1,680)  | 1:41:A:ALA:H    | 1:36:A:VAL:HG23  | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,537)  | 1:54:A:LYS:HB2  | 1:60:A:GLN:HB3  | 19       | 0.15          |
| (1,471)  | 1:84:A:GLU:H    | 1:86:A:LEU:HD23 | 16       | 0.15          |
| (1,402)  | 1:32:A:ILE:HD12 | 1:121:A:PRO:HG2 | 2        | 0.15          |
| (1,402)  | 1:32:A:ILE:HD11 | 1:121:A:PRO:HG2 | 2        | 0.15          |
| (1,402)  | 1:32:A:ILE:HD13 | 1:121:A:PRO:HG2 | 2        | 0.15          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE1  | 17       | 0.15          |
| (1,384)  | 1:31:A:PRO:HB3  | 1:10:A:PHE:HE2  | 17       | 0.15          |
| (1,351)  | 1:130:A:TYR:H   | 1:129:A:GLY:HA2 | 10       | 0.15          |
| (1,351)  | 1:130:A:TYR:H   | 1:129:A:GLY:HA2 | 15       | 0.15          |
| (1,315)  | 1:74:A:THR:H    | 1:73:A:GLY:HA2  | 12       | 0.15          |
| (1,221)  | 1:111:A:THR:H   | 1:110:A:PRO:HG3 | 2        | 0.15          |
| (1,123)  | 1:22:A:PHE:H    | 1:21:A:ASP:HA   | 13       | 0.15          |
| (1,123)  | 1:22:A:PHE:H    | 1:21:A:ASP:HA   | 18       | 0.15          |
| (1,121)  | 1:68:A:TYR:HE1  | 1:66:A:ARG:HB2  | 3        | 0.15          |
| (1,121)  | 1:68:A:TYR:HE2  | 1:66:A:ARG:HB2  | 3        | 0.15          |
| (1,104)  | 1:108:A:ARG:H   | 1:106:A:SER:HA  | 15       | 0.15          |
| (1,93)   | 1:4:A:ILE:HB    | 1:5:A:PRO:HD3   | 3        | 0.15          |
| (1,93)   | 1:4:A:ILE:HB    | 1:5:A:PRO:HD3   | 11       | 0.15          |
| (1,83)   | 1:46:A:TYR:HD1  | 1:76:A:PRO:HD3  | 16       | 0.15          |
| (1,83)   | 1:46:A:TYR:HD2  | 1:76:A:PRO:HD3  | 16       | 0.15          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3  | 2        | 0.15          |
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB   | 19       | 0.14          |
| (2,1182) | 1:92:A:VAL:CB   | 1:30:A:VAL:CB   | 11       | 0.14          |
| (2,1116) | 1:82:A:TYR:CA   | 1:72:A:LEU:CB   | 4        | 0.14          |
| (2,1116) | 1:82:A:TYR:CA   | 1:72:A:LEU:CB   | 7        | 0.14          |
| (2,1091) | 1:103:A:SER:H   | 1:72:A:LEU:H    | 6        | 0.14          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB   | 16       | 0.14          |
| (2,980)  | 1:124:A:THR:H   | 1:28:A:GLN:CB   | 17       | 0.14          |
| (2,891)  | 1:48:A:HIS:CB   | 1:68:A:TYR:CB   | 12       | 0.14          |
| (2,853)  | 1:6:A:HIS:CB    | 1:4:A:ILE:CB    | 5        | 0.14          |
| (2,853)  | 1:6:A:HIS:CB    | 1:4:A:ILE:CB    | 15       | 0.14          |
| (2,722)  | 1:114:A:GLU:CB  | 1:115:A:ALA:CB  | 16       | 0.14          |
| (2,685)  | 1:103:A:SER:H   | 1:105:A:VAL:CB  | 1        | 0.14          |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB   | 2        | 0.14          |
| (2,643)  | 1:68:A:TYR:H    | 1:48:A:HIS:H    | 8        | 0.14          |
| (2,643)  | 1:68:A:TYR:H    | 1:48:A:HIS:H    | 15       | 0.14          |
| (2,571)  | 1:89:A:VAL:CB   | 1:45:A:TRP:CB   | 6        | 0.14          |
| (2,481)  | 1:118:A:THR:H   | 1:11:A:SER:H    | 12       | 0.14          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 1        | 0.14          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 6        | 0.14          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB   | 12       | 0.14          |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H    | 7        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,469)  | 1:44:A:TYR:H     | 1:72:A:LEU:H     | 11       | 0.14          |
| (2,469)  | 1:44:A:TYR:H     | 1:72:A:LEU:H     | 15       | 0.14          |
| (2,440)  | 1:91:A:TRP:H     | 1:89:A:VAL:CB    | 18       | 0.14          |
| (2,431)  | 1:120:A:PHE:H    | 1:32:A:ILE:CB    | 2        | 0.14          |
| (2,156)  | 1:4:A:ILE:CB     | 1:6:A:HIS:CB     | 18       | 0.14          |
| (2,130)  | 1:120:A:PHE:CB   | 1:30:A:VAL:CA    | 11       | 0.14          |
| (2,84)   | 1:44:A:TYR:CB    | 1:91:A:TRP:CB    | 8        | 0.14          |
| (2,74)   | 1:13:A:ILE:CA    | 1:133:A:GLU:H    | 6        | 0.14          |
| (2,33)   | 1:104:A:ASP:H    | 1:105:A:VAL:CB   | 10       | 0.14          |
| (1,1252) | 1:121:A:PRO:HA   | 1:32:A:ILE:HG12  | 18       | 0.14          |
| (1,1243) | 1:113:A:GLN:HG3  | 1:110:A:PRO:HB2  | 15       | 0.14          |
| (1,1243) | 1:113:A:GLN:HG2  | 1:110:A:PRO:HB2  | 15       | 0.14          |
| (1,1228) | 1:103:A:SER:H    | 1:72:A:LEU:H     | 6        | 0.14          |
| (1,1220) | 1:103:A:SER:HA   | 1:72:A:LEU:HD21  | 16       | 0.14          |
| (1,1210) | 1:43:A:GLY:H     | 1:92:A:VAL:HB    | 11       | 0.14          |
| (1,1199) | 1:9:A:TRP:HE1    | 1:108:A:ARG:HD3  | 3        | 0.14          |
| (1,1167) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2   | 4        | 0.14          |
| (1,1167) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2   | 17       | 0.14          |
| (1,1162) | 1:62:A:GLN:HG2   | 1:63:A:LEU:HG    | 5        | 0.14          |
| (1,1144) | 1:51:A:ARG:HA    | 1:52:A:SER:HB3   | 10       | 0.14          |
| (1,1142) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2   | 4        | 0.14          |
| (1,1142) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2   | 17       | 0.14          |
| (1,1043) | 1:51:A:ARG:HB3   | 1:52:A:SER:HA    | 11       | 0.14          |
| (1,1014) | 1:62:A:GLN:HA    | 1:52:A:SER:HA    | 8        | 0.14          |
| (1,1008) | 1:116:A:ILE:HA   | 1:117:A:PRO:HD2  | 17       | 0.14          |
| (1,927)  | 1:71:A:TYR:HE2   | 1:105:A:VAL:HG23 | 16       | 0.14          |
| (1,873)  | 1:78:A:ALA:H     | 1:76:A:PRO:HD3   | 11       | 0.14          |
| (1,833)  | 1:118:A:THR:H    | 1:117:A:PRO:HG2  | 7        | 0.14          |
| (1,768)  | 1:119:A:ARG:H    | 1:31:A:PRO:HB3   | 13       | 0.14          |
| (1,725)  | 1:72:A:LEU:H     | 1:102:A:PRO:HA   | 3        | 0.14          |
| (1,725)  | 1:72:A:LEU:H     | 1:102:A:PRO:HA   | 19       | 0.14          |
| (1,715)  | 1:105:A:VAL:HG12 | 1:103:A:SER:HB2  | 13       | 0.14          |
| (1,715)  | 1:105:A:VAL:HG11 | 1:103:A:SER:HB2  | 13       | 0.14          |
| (1,715)  | 1:105:A:VAL:HG13 | 1:103:A:SER:HB2  | 13       | 0.14          |
| (1,712)  | 1:68:A:TYR:H     | 1:48:A:HIS:H     | 8        | 0.14          |
| (1,712)  | 1:68:A:TYR:H     | 1:48:A:HIS:H     | 15       | 0.14          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 3        | 0.14          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 12       | 0.14          |
| (1,706)  | 1:61:A:LYS:H     | 1:60:A:GLN:HB2   | 1        | 0.14          |
| (1,706)  | 1:61:A:LYS:H     | 1:60:A:GLN:HB2   | 6        | 0.14          |
| (1,702)  | 1:58:A:GLY:H     | 1:57:A:ASP:HB3   | 6        | 0.14          |
| (1,680)  | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 6        | 0.14          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,680) | 1:41:A:ALA:H     | 1:36:A:VAL:HG23 | 8        | 0.14          |
| (1,654) | 1:16:A:PHE:H     | 1:64:A:LEU:HD23 | 11       | 0.14          |
| (1,653) | 1:16:A:PHE:H     | 1:64:A:LEU:HD21 | 3        | 0.14          |
| (1,653) | 1:16:A:PHE:H     | 1:64:A:LEU:HD21 | 6        | 0.14          |
| (1,653) | 1:16:A:PHE:H     | 1:64:A:LEU:HD21 | 8        | 0.14          |
| (1,599) | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD22 | 17       | 0.14          |
| (1,537) | 1:54:A:LYS:HB2   | 1:60:A:GLN:HB3  | 9        | 0.14          |
| (1,521) | 1:118:A:THR:H    | 1:11:A:SER:H    | 12       | 0.14          |
| (1,509) | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 7        | 0.14          |
| (1,509) | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 11       | 0.14          |
| (1,509) | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 15       | 0.14          |
| (1,471) | 1:84:A:GLU:H     | 1:86:A:LEU:HD23 | 10       | 0.14          |
| (1,471) | 1:84:A:GLU:H     | 1:86:A:LEU:HD23 | 17       | 0.14          |
| (1,414) | 1:65:A:PRO:HB3   | 1:67:A:TRP:HE1  | 17       | 0.14          |
| (1,402) | 1:32:A:ILE:HD12  | 1:121:A:PRO:HG2 | 12       | 0.14          |
| (1,402) | 1:32:A:ILE:HD11  | 1:121:A:PRO:HG2 | 12       | 0.14          |
| (1,402) | 1:32:A:ILE:HD13  | 1:121:A:PRO:HG2 | 12       | 0.14          |
| (1,402) | 1:32:A:ILE:HD12  | 1:121:A:PRO:HG2 | 15       | 0.14          |
| (1,402) | 1:32:A:ILE:HD11  | 1:121:A:PRO:HG2 | 15       | 0.14          |
| (1,402) | 1:32:A:ILE:HD13  | 1:121:A:PRO:HG2 | 15       | 0.14          |
| (1,385) | 1:118:A:THR:H    | 1:117:A:PRO:HB2 | 2        | 0.14          |
| (1,385) | 1:118:A:THR:H    | 1:117:A:PRO:HB2 | 4        | 0.14          |
| (1,349) | 1:63:A:LEU:H     | 1:52:A:SER:HB2  | 15       | 0.14          |
| (1,315) | 1:74:A:THR:H     | 1:73:A:GLY:HA2  | 5        | 0.14          |
| (1,288) | 1:16:A:PHE:HA    | 1:64:A:LEU:HD23 | 16       | 0.14          |
| (1,229) | 1:59:A:GLN:HA    | 1:54:A:LYS:HB3  | 10       | 0.14          |
| (1,221) | 1:111:A:THR:H    | 1:110:A:PRO:HG3 | 3        | 0.14          |
| (1,204) | 1:125:A:ILE:HG12 | 1:23:A:LYS:HB3  | 10       | 0.14          |
| (1,200) | 1:115:A:ALA:H    | 1:114:A:GLU:HB3 | 18       | 0.14          |
| (1,138) | 1:138:A:SER:H    | 1:137:A:ARG:HA  | 8        | 0.14          |
| (1,125) | 1:5:A:PRO:HD3    | 1:4:A:ILE:HG23  | 6        | 0.14          |
| (1,125) | 1:5:A:PRO:HD3    | 1:4:A:ILE:HG23  | 13       | 0.14          |
| (1,123) | 1:22:A:PHE:H     | 1:21:A:ASP:HA   | 5        | 0.14          |
| (1,123) | 1:22:A:PHE:H     | 1:21:A:ASP:HA   | 19       | 0.14          |
| (1,110) | 1:32:A:ILE:HG23  | 1:121:A:PRO:HG2 | 7        | 0.14          |
| (1,93)  | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 7        | 0.14          |
| (1,93)  | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 8        | 0.14          |
| (1,93)  | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 16       | 0.14          |
| (1,93)  | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 18       | 0.14          |
| (1,83)  | 1:46:A:TYR:HD1   | 1:76:A:PRO:HD3  | 5        | 0.14          |
| (1,83)  | 1:46:A:TYR:HD2   | 1:76:A:PRO:HD3  | 5        | 0.14          |
| (1,81)  | 1:13:A:ILE:HA    | 1:133:A:GLU:H   | 6        | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,54)   | 1:63:A:LEU:HA  | 1:62:A:GLN:HG2 | 11       | 0.14          |
| (2,1159) | 1:96:A:GLN:CB  | 1:38:A:PRO:CB  | 18       | 0.13          |
| (2,1124) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB  | 12       | 0.13          |
| (2,1111) | 1:14:A:THR:CA  | 1:66:A:ARG:CB  | 19       | 0.13          |
| (2,1091) | 1:103:A:SER:H  | 1:72:A:LEU:H   | 12       | 0.13          |
| (2,1091) | 1:103:A:SER:H  | 1:72:A:LEU:H   | 13       | 0.13          |
| (2,1091) | 1:103:A:SER:H  | 1:72:A:LEU:H   | 17       | 0.13          |
| (2,1077) | 1:43:A:GLY:H   | 1:72:A:LEU:CB  | 8        | 0.13          |
| (2,1044) | 1:51:A:ARG:CB  | 1:63:A:LEU:CB  | 12       | 0.13          |
| (2,1034) | 1:113:A:GLN:CB | 1:9:A:TRP:CA   | 14       | 0.13          |
| (2,888)  | 1:5:A:PRO:CB   | 1:6:A:HIS:CB   | 10       | 0.13          |
| (2,887)  | 1:66:A:ARG:CB  | 1:68:A:TYR:CB  | 11       | 0.13          |
| (2,885)  | 1:32:A:ILE:CB  | 1:120:A:PHE:CB | 14       | 0.13          |
| (2,865)  | 1:66:A:ARG:CB  | 1:68:A:TYR:CB  | 11       | 0.13          |
| (2,777)  | 1:25:A:SER:H   | 1:29:A:GLY:H   | 10       | 0.13          |
| (2,718)  | 1:42:A:LYS:H   | 1:40:A:GLU:CB  | 8        | 0.13          |
| (2,685)  | 1:103:A:SER:H  | 1:105:A:VAL:CB | 16       | 0.13          |
| (2,657)  | 1:72:A:LEU:H   | 1:42:A:LYS:CB  | 16       | 0.13          |
| (2,593)  | 1:16:A:PHE:H   | 1:64:A:LEU:CB  | 15       | 0.13          |
| (2,538)  | 1:13:A:ILE:H   | 1:69:A:PHE:CB  | 1        | 0.13          |
| (2,538)  | 1:13:A:ILE:H   | 1:69:A:PHE:CB  | 18       | 0.13          |
| (2,471)  | 1:41:A:ALA:CB  | 1:94:A:ASN:CB  | 10       | 0.13          |
| (2,471)  | 1:41:A:ALA:CB  | 1:94:A:ASN:CB  | 13       | 0.13          |
| (2,471)  | 1:41:A:ALA:CB  | 1:94:A:ASN:CB  | 14       | 0.13          |
| (2,469)  | 1:44:A:TYR:H   | 1:72:A:LEU:H   | 3        | 0.13          |
| (2,469)  | 1:44:A:TYR:H   | 1:72:A:LEU:H   | 6        | 0.13          |
| (2,469)  | 1:44:A:TYR:H   | 1:72:A:LEU:H   | 8        | 0.13          |
| (2,469)  | 1:44:A:TYR:H   | 1:72:A:LEU:H   | 12       | 0.13          |
| (2,469)  | 1:44:A:TYR:H   | 1:72:A:LEU:H   | 16       | 0.13          |
| (2,466)  | 1:41:A:ALA:CA  | 1:30:A:VAL:CB  | 8        | 0.13          |
| (2,466)  | 1:41:A:ALA:CA  | 1:30:A:VAL:CB  | 10       | 0.13          |
| (2,466)  | 1:41:A:ALA:CA  | 1:30:A:VAL:CB  | 14       | 0.13          |
| (2,459)  | 1:13:A:ILE:H   | 1:133:A:GLU:H  | 1        | 0.13          |
| (2,451)  | 1:43:A:GLY:H   | 1:92:A:VAL:H   | 14       | 0.13          |
| (2,451)  | 1:43:A:GLY:H   | 1:92:A:VAL:H   | 15       | 0.13          |
| (2,431)  | 1:120:A:PHE:H  | 1:32:A:ILE:CB  | 12       | 0.13          |
| (2,369)  | 1:96:A:GLN:CB  | 1:38:A:PRO:CB  | 2        | 0.13          |
| (2,362)  | 1:104:A:ASP:H  | 1:40:A:GLU:CB  | 15       | 0.13          |
| (2,361)  | 1:81:A:SER:H   | 1:84:A:GLU:CB  | 15       | 0.13          |
| (2,263)  | 1:16:A:PHE:CA  | 1:64:A:LEU:CB  | 18       | 0.13          |
| (2,261)  | 1:108:A:ARG:H  | 1:107:A:SER:H  | 7        | 0.13          |
| (2,261)  | 1:108:A:ARG:H  | 1:107:A:SER:H  | 11       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,128)  | 1:28:A:GLN:CA    | 1:120:A:PHE:CB   | 8        | 0.13          |
| (2,128)  | 1:28:A:GLN:CA    | 1:120:A:PHE:CB   | 17       | 0.13          |
| (2,102)  | 1:48:A:HIS:CB    | 1:68:A:TYR:CB    | 16       | 0.13          |
| (2,74)   | 1:13:A:ILE:CA    | 1:133:A:GLU:H    | 10       | 0.13          |
| (2,33)   | 1:104:A:ASP:H    | 1:105:A:VAL:CB   | 12       | 0.13          |
| (2,3)    | 1:46:A:TYR:CB    | 1:76:A:PRO:CB    | 10       | 0.13          |
| (1,1272) | 1:129:A:GLY:HA3  | 1:17:A:GLN:HB2   | 4        | 0.13          |
| (1,1256) | 1:27:A:GLY:H     | 1:28:A:GLN:HB3   | 11       | 0.13          |
| (1,1228) | 1:103:A:SER:H    | 1:72:A:LEU:H     | 12       | 0.13          |
| (1,1228) | 1:103:A:SER:H    | 1:72:A:LEU:H     | 13       | 0.13          |
| (1,1228) | 1:103:A:SER:H    | 1:72:A:LEU:H     | 17       | 0.13          |
| (1,1220) | 1:103:A:SER:HA   | 1:72:A:LEU:HD21  | 4        | 0.13          |
| (1,1210) | 1:43:A:GLY:H     | 1:92:A:VAL:HB    | 2        | 0.13          |
| (1,1167) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2   | 19       | 0.13          |
| (1,1165) | 1:60:A:GLN:HG2   | 1:54:A:LYS:HB2   | 18       | 0.13          |
| (1,1159) | 1:127:A:PRO:HA   | 1:128:A:GLN:HG3  | 17       | 0.13          |
| (1,1156) | 1:63:A:LEU:HA    | 1:62:A:GLN:HB2   | 2        | 0.13          |
| (1,1156) | 1:63:A:LEU:HA    | 1:62:A:GLN:HB2   | 16       | 0.13          |
| (1,1142) | 1:51:A:ARG:HA    | 1:52:A:SER:HB2   | 19       | 0.13          |
| (1,1139) | 1:51:A:ARG:HA    | 1:52:A:SER:H     | 11       | 0.13          |
| (1,1120) | 1:130:A:TYR:H    | 1:13:A:ILE:HG23  | 7        | 0.13          |
| (1,924)  | 1:71:A:TYR:HD2   | 1:105:A:VAL:HG23 | 10       | 0.13          |
| (1,924)  | 1:71:A:TYR:HD2   | 1:105:A:VAL:HG23 | 13       | 0.13          |
| (1,924)  | 1:71:A:TYR:HD2   | 1:105:A:VAL:HG23 | 15       | 0.13          |
| (1,924)  | 1:71:A:TYR:HD2   | 1:105:A:VAL:HG23 | 16       | 0.13          |
| (1,924)  | 1:71:A:TYR:HD2   | 1:105:A:VAL:HG23 | 19       | 0.13          |
| (1,887)  | 1:129:A:GLY:HA3  | 1:128:A:GLN:HG3  | 4        | 0.13          |
| (1,854)  | 1:25:A:SER:H     | 1:29:A:GLY:H     | 10       | 0.13          |
| (1,805)  | 1:117:A:PRO:HA   | 1:11:A:SER:HA    | 19       | 0.13          |
| (1,790)  | 1:42:A:LYS:H     | 1:40:A:GLU:HB2   | 19       | 0.13          |
| (1,768)  | 1:119:A:ARG:H    | 1:31:A:PRO:HB3   | 18       | 0.13          |
| (1,745)  | 1:91:A:TRP:H     | 1:90:A:PHE:HB3   | 1        | 0.13          |
| (1,715)  | 1:105:A:VAL:HG12 | 1:103:A:SER:HB2  | 11       | 0.13          |
| (1,715)  | 1:105:A:VAL:HG11 | 1:103:A:SER:HB2  | 11       | 0.13          |
| (1,715)  | 1:105:A:VAL:HG13 | 1:103:A:SER:HB2  | 11       | 0.13          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 4        | 0.13          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 11       | 0.13          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 15       | 0.13          |
| (1,706)  | 1:61:A:LYS:H     | 1:60:A:GLN:HB2   | 18       | 0.13          |
| (1,653)  | 1:16:A:PHE:H     | 1:64:A:LEU:HD21  | 10       | 0.13          |
| (1,626)  | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 18       | 0.13          |
| (1,509)  | 1:44:A:TYR:H     | 1:72:A:LEU:H     | 3        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,509)  | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 6        | 0.13          |
| (1,509)  | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 8        | 0.13          |
| (1,509)  | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 12       | 0.13          |
| (1,509)  | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 16       | 0.13          |
| (1,499)  | 1:13:A:ILE:H     | 1:133:A:GLU:H   | 1        | 0.13          |
| (1,491)  | 1:43:A:GLY:H     | 1:92:A:VAL:H    | 14       | 0.13          |
| (1,491)  | 1:43:A:GLY:H     | 1:92:A:VAL:H    | 15       | 0.13          |
| (1,414)  | 1:65:A:PRO:HB3   | 1:67:A:TRP:HE1  | 1        | 0.13          |
| (1,385)  | 1:118:A:THR:H    | 1:117:A:PRO:HB2 | 1        | 0.13          |
| (1,385)  | 1:118:A:THR:H    | 1:117:A:PRO:HB2 | 15       | 0.13          |
| (1,355)  | 1:82:A:TYR:H     | 1:81:A:SER:HB3  | 5        | 0.13          |
| (1,351)  | 1:130:A:TYR:H    | 1:129:A:GLY:HA2 | 11       | 0.13          |
| (1,349)  | 1:63:A:LEU:H     | 1:52:A:SER:HB2  | 16       | 0.13          |
| (1,324)  | 1:73:A:GLY:H     | 1:74:A:THR:HB   | 2        | 0.13          |
| (1,284)  | 1:108:A:ARG:H    | 1:107:A:SER:H   | 7        | 0.13          |
| (1,284)  | 1:108:A:ARG:H    | 1:107:A:SER:H   | 11       | 0.13          |
| (1,257)  | 1:116:A:ILE:HG23 | 1:10:A:PHE:HA   | 6        | 0.13          |
| (1,221)  | 1:111:A:THR:H    | 1:110:A:PRO:HG3 | 8        | 0.13          |
| (1,114)  | 1:104:A:ASP:H    | 1:103:A:SER:HA  | 11       | 0.13          |
| (1,109)  | 1:32:A:ILE:HG22  | 1:121:A:PRO:HG2 | 7        | 0.13          |
| (1,109)  | 1:32:A:ILE:HG21  | 1:121:A:PRO:HG2 | 7        | 0.13          |
| (1,93)   | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 9        | 0.13          |
| (1,93)   | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 12       | 0.13          |
| (1,93)   | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 14       | 0.13          |
| (1,93)   | 1:4:A:ILE:HB     | 1:5:A:PRO:HD3   | 15       | 0.13          |
| (1,87)   | 1:113:A:GLN:HE21 | 1:9:A:TRP:HD1   | 8        | 0.13          |
| (1,87)   | 1:113:A:GLN:HE21 | 1:9:A:TRP:HD1   | 17       | 0.13          |
| (1,54)   | 1:63:A:LEU:HA    | 1:62:A:GLN:HG2  | 6        | 0.13          |
| (1,47)   | 1:25:A:SER:HA    | 1:28:A:GLN:HB3  | 14       | 0.13          |
| (1,26)   | 1:115:A:ALA:H    | 1:114:A:GLU:HG2 | 17       | 0.13          |
| (1,6)    | 1:44:A:TYR:H     | 1:91:A:TRP:HZ3  | 17       | 0.13          |
| (2,1201) | 1:52:A:SER:CB    | 1:62:A:GLN:CB   | 13       | 0.12          |
| (2,1126) | 1:20:A:ARG:CB    | 1:128:A:GLN:CB  | 2        | 0.12          |
| (2,1112) | 1:121:A:PRO:CA   | 1:32:A:ILE:CB   | 7        | 0.12          |
| (2,1091) | 1:103:A:SER:H    | 1:72:A:LEU:H    | 1        | 0.12          |
| (2,1091) | 1:103:A:SER:H    | 1:72:A:LEU:H    | 10       | 0.12          |
| (2,982)  | 1:124:A:THR:H    | 1:125:A:ILE:CB  | 19       | 0.12          |
| (2,980)  | 1:124:A:THR:H    | 1:28:A:GLN:CB   | 18       | 0.12          |
| (2,945)  | 1:22:A:PHE:CA    | 1:127:A:PRO:CB  | 1        | 0.12          |
| (2,885)  | 1:32:A:ILE:CB    | 1:120:A:PHE:CB  | 2        | 0.12          |
| (2,885)  | 1:32:A:ILE:CB    | 1:120:A:PHE:CB  | 6        | 0.12          |
| (2,885)  | 1:32:A:ILE:CB    | 1:120:A:PHE:CB  | 7        | 0.12          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB   | 6        | 0.12          |
| (2,817)  | 1:132:A:VAL:CB | 1:126:A:LEU:CB   | 6        | 0.12          |
| (2,782)  | 1:124:A:THR:CB | 1:28:A:GLN:CB    | 17       | 0.12          |
| (2,777)  | 1:25:A:SER:H   | 1:29:A:GLY:H     | 13       | 0.12          |
| (2,699)  | 1:111:A:THR:CB | 1:110:A:PRO:CB   | 3        | 0.12          |
| (2,699)  | 1:111:A:THR:CB | 1:110:A:PRO:CB   | 19       | 0.12          |
| (2,698)  | 1:120:A:PHE:H  | 1:132:A:VAL:CB   | 10       | 0.12          |
| (2,635)  | 1:59:A:GLN:H   | 1:54:A:LYS:CB    | 1        | 0.12          |
| (2,560)  | 1:84:A:GLU:H   | 1:91:A:TRP:CB    | 5        | 0.12          |
| (2,560)  | 1:84:A:GLU:H   | 1:91:A:TRP:CB    | 16       | 0.12          |
| (2,538)  | 1:13:A:ILE:H   | 1:69:A:PHE:CB    | 2        | 0.12          |
| (2,471)  | 1:41:A:ALA:CB  | 1:94:A:ASN:CB    | 16       | 0.12          |
| (2,469)  | 1:44:A:TYR:H   | 1:72:A:LEU:H     | 19       | 0.12          |
| (2,451)  | 1:43:A:GLY:H   | 1:92:A:VAL:H     | 4        | 0.12          |
| (2,451)  | 1:43:A:GLY:H   | 1:92:A:VAL:H     | 17       | 0.12          |
| (2,444)  | 1:104:A:ASP:CB | 1:36:A:VAL:CB    | 6        | 0.12          |
| (2,431)  | 1:120:A:PHE:H  | 1:32:A:ILE:CB    | 3        | 0.12          |
| (2,431)  | 1:120:A:PHE:H  | 1:32:A:ILE:CB    | 15       | 0.12          |
| (2,404)  | 1:71:A:TYR:H   | 1:74:A:THR:CB    | 4        | 0.12          |
| (2,74)   | 1:13:A:ILE:CA  | 1:133:A:GLU:H    | 14       | 0.12          |
| (2,68)   | 1:86:A:LEU:H   | 1:45:A:TRP:CB    | 13       | 0.12          |
| (2,33)   | 1:104:A:ASP:H  | 1:105:A:VAL:CB   | 6        | 0.12          |
| (2,30)   | 1:16:A:PHE:H   | 1:17:A:GLN:CB    | 7        | 0.12          |
| (1,1256) | 1:27:A:GLY:H   | 1:28:A:GLN:HB3   | 19       | 0.12          |
| (1,1236) | 1:138:A:SER:HA | 1:11:A:SER:HB3   | 7        | 0.12          |
| (1,1228) | 1:103:A:SER:H  | 1:72:A:LEU:H     | 1        | 0.12          |
| (1,1228) | 1:103:A:SER:H  | 1:72:A:LEU:H     | 10       | 0.12          |
| (1,1211) | 1:43:A:GLY:H   | 1:72:A:LEU:HB3   | 8        | 0.12          |
| (1,1167) | 1:51:A:ARG:HA  | 1:52:A:SER:HB2   | 14       | 0.12          |
| (1,1167) | 1:51:A:ARG:HA  | 1:52:A:SER:HB2   | 18       | 0.12          |
| (1,1142) | 1:51:A:ARG:HA  | 1:52:A:SER:HB2   | 14       | 0.12          |
| (1,1142) | 1:51:A:ARG:HA  | 1:52:A:SER:HB2   | 18       | 0.12          |
| (1,1128) | 1:73:A:GLY:HA3 | 1:102:A:PRO:HG2  | 13       | 0.12          |
| (1,1013) | 1:64:A:LEU:H   | 1:63:A:LEU:HG    | 7        | 0.12          |
| (1,1007) | 1:5:A:PRO:HD2  | 1:4:A:ILE:HA     | 2        | 0.12          |
| (1,955)  | 1:13:A:ILE:HA  | 1:66:A:ARG:HG2   | 3        | 0.12          |
| (1,955)  | 1:13:A:ILE:HA  | 1:66:A:ARG:HG2   | 14       | 0.12          |
| (1,927)  | 1:71:A:TYR:HE2 | 1:105:A:VAL:HG23 | 4        | 0.12          |
| (1,924)  | 1:71:A:TYR:HD2 | 1:105:A:VAL:HG23 | 2        | 0.12          |
| (1,924)  | 1:71:A:TYR:HD2 | 1:105:A:VAL:HG23 | 6        | 0.12          |
| (1,924)  | 1:71:A:TYR:HD2 | 1:105:A:VAL:HG23 | 7        | 0.12          |
| (1,924)  | 1:71:A:TYR:HD2 | 1:105:A:VAL:HG23 | 9        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,924) | 1:71:A:TYR:HD2   | 1:105:A:VAL:HG23 | 12       | 0.12          |
| (1,854) | 1:25:A:SER:H     | 1:29:A:GLY:H     | 13       | 0.12          |
| (1,833) | 1:118:A:THR:H    | 1:117:A:PRO:HG2  | 16       | 0.12          |
| (1,768) | 1:119:A:ARG:H    | 1:31:A:PRO:HB3   | 9        | 0.12          |
| (1,745) | 1:91:A:TRP:H     | 1:90:A:PHE:HB3   | 13       | 0.12          |
| (1,745) | 1:91:A:TRP:H     | 1:90:A:PHE:HB3   | 18       | 0.12          |
| (1,715) | 1:105:A:VAL:HG12 | 1:103:A:SER:HB2  | 1        | 0.12          |
| (1,715) | 1:105:A:VAL:HG11 | 1:103:A:SER:HB2  | 1        | 0.12          |
| (1,715) | 1:105:A:VAL:HG13 | 1:103:A:SER:HB2  | 1        | 0.12          |
| (1,711) | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 10       | 0.12          |
| (1,711) | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 17       | 0.12          |
| (1,680) | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 9        | 0.12          |
| (1,680) | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 10       | 0.12          |
| (1,680) | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 15       | 0.12          |
| (1,653) | 1:16:A:PHE:H     | 1:64:A:LEU:HD21  | 4        | 0.12          |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 2        | 0.12          |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 9        | 0.12          |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 17       | 0.12          |
| (1,621) | 1:89:A:VAL:HG12  | 1:86:A:LEU:HD22  | 5        | 0.12          |
| (1,599) | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD22  | 18       | 0.12          |
| (1,509) | 1:44:A:TYR:H     | 1:72:A:LEU:H     | 19       | 0.12          |
| (1,508) | 1:41:A:ALA:HA    | 1:71:A:TYR:HE2   | 18       | 0.12          |
| (1,491) | 1:43:A:GLY:H     | 1:92:A:VAL:H     | 4        | 0.12          |
| (1,491) | 1:43:A:GLY:H     | 1:92:A:VAL:H     | 17       | 0.12          |
| (1,485) | 1:40:A:GLU:HB3   | 1:36:A:VAL:HG23  | 16       | 0.12          |
| (1,471) | 1:84:A:GLU:H     | 1:86:A:LEU:HD23  | 13       | 0.12          |
| (1,414) | 1:65:A:PRO:HB3   | 1:67:A:TRP:HE1   | 7        | 0.12          |
| (1,385) | 1:118:A:THR:H    | 1:117:A:PRO:HB2  | 10       | 0.12          |
| (1,348) | 1:27:A:GLY:HA2   | 1:94:A:ASN:HA    | 18       | 0.12          |
| (1,347) | 1:89:A:VAL:H     | 1:88:A:GLY:HA3   | 17       | 0.12          |
| (1,315) | 1:74:A:THR:H     | 1:73:A:GLY:HA2   | 10       | 0.12          |
| (1,315) | 1:74:A:THR:H     | 1:73:A:GLY:HA2   | 13       | 0.12          |
| (1,302) | 1:43:A:GLY:HA3   | 1:72:A:LEU:H     | 12       | 0.12          |
| (1,288) | 1:16:A:PHE:HA    | 1:64:A:LEU:HD23  | 14       | 0.12          |
| (1,259) | 1:10:A:PHE:HA    | 1:8:A:SER:HA     | 8        | 0.12          |
| (1,259) | 1:10:A:PHE:HA    | 1:8:A:SER:HA     | 15       | 0.12          |
| (1,198) | 1:18:A:LYS:HG2   | 1:64:A:LEU:HD12  | 12       | 0.12          |
| (1,198) | 1:18:A:LYS:HG2   | 1:64:A:LEU:HD11  | 12       | 0.12          |
| (1,198) | 1:18:A:LYS:HG2   | 1:64:A:LEU:HD13  | 12       | 0.12          |
| (1,175) | 1:82:A:TYR:H     | 1:81:A:SER:HB2   | 19       | 0.12          |
| (1,138) | 1:138:A:SER:H    | 1:137:A:ARG:HA   | 15       | 0.12          |
| (1,125) | 1:5:A:PRO:HD3    | 1:4:A:ILE:HG23   | 4        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,125)  | 1:5:A:PRO:HD3   | 1:4:A:ILE:HG23   | 10       | 0.12          |
| (1,121)  | 1:68:A:TYR:HE1  | 1:66:A:ARG:HB2   | 9        | 0.12          |
| (1,121)  | 1:68:A:TYR:HE2  | 1:66:A:ARG:HB2   | 9        | 0.12          |
| (1,120)  | 1:24:A:PHE:HA   | 1:125:A:ILE:HG23 | 14       | 0.12          |
| (1,93)   | 1:4:A:ILE:HB    | 1:5:A:PRO:HD3    | 5        | 0.12          |
| (1,81)   | 1:13:A:ILE:HA   | 1:133:A:GLU:H    | 1        | 0.12          |
| (1,81)   | 1:13:A:ILE:HA   | 1:133:A:GLU:H    | 12       | 0.12          |
| (1,54)   | 1:63:A:LEU:HA   | 1:62:A:GLN:HG2   | 10       | 0.12          |
| (1,49)   | 1:89:A:VAL:HG23 | 1:45:A:TRP:HD1   | 2        | 0.12          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3   | 1        | 0.12          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3   | 13       | 0.12          |
| (2,1138) | 1:103:A:SER:CA  | 1:42:A:LYS:CB    | 8        | 0.11          |
| (2,1112) | 1:121:A:PRO:CA  | 1:32:A:ILE:CB    | 4        | 0.11          |
| (2,1059) | 1:48:A:HIS:H    | 1:46:A:TYR:CB    | 8        | 0.11          |
| (2,987)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB   | 5        | 0.11          |
| (2,987)  | 1:32:A:ILE:CB   | 1:121:A:PRO:CB   | 10       | 0.11          |
| (2,887)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB    | 8        | 0.11          |
| (2,865)  | 1:66:A:ARG:CB   | 1:68:A:TYR:CB    | 8        | 0.11          |
| (2,777)  | 1:25:A:SER:H    | 1:29:A:GLY:H     | 2        | 0.11          |
| (2,777)  | 1:25:A:SER:H    | 1:29:A:GLY:H     | 11       | 0.11          |
| (2,705)  | 1:125:A:ILE:H   | 1:25:A:SER:CB    | 1        | 0.11          |
| (2,705)  | 1:125:A:ILE:H   | 1:25:A:SER:CB    | 19       | 0.11          |
| (2,697)  | 1:119:A:ARG:H   | 1:31:A:PRO:CB    | 9        | 0.11          |
| (2,685)  | 1:103:A:SER:H   | 1:105:A:VAL:CB   | 15       | 0.11          |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB    | 6        | 0.11          |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB    | 9        | 0.11          |
| (2,657)  | 1:72:A:LEU:H    | 1:42:A:LYS:CB    | 13       | 0.11          |
| (2,606)  | 1:32:A:ILE:CB   | 1:34:A:PHE:H     | 2        | 0.11          |
| (2,538)  | 1:13:A:ILE:H    | 1:69:A:PHE:CB    | 5        | 0.11          |
| (2,510)  | 1:100:A:SER:H   | 1:99:A:THR:H     | 1        | 0.11          |
| (2,471)  | 1:41:A:ALA:CB   | 1:94:A:ASN:CB    | 4        | 0.11          |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H     | 2        | 0.11          |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H     | 9        | 0.11          |
| (2,466)  | 1:41:A:ALA:CA   | 1:30:A:VAL:CB    | 19       | 0.11          |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 13       | 0.11          |
| (2,418)  | 1:45:A:TRP:H    | 1:92:A:VAL:CB    | 11       | 0.11          |
| (2,396)  | 1:15:A:GLN:H    | 1:64:A:LEU:CB    | 1        | 0.11          |
| (2,385)  | 1:16:A:PHE:H    | 1:64:A:LEU:CB    | 8        | 0.11          |
| (2,369)  | 1:96:A:GLN:CB   | 1:38:A:PRO:CB    | 11       | 0.11          |
| (2,255)  | 1:112:A:THR:H   | 1:109:A:ASP:H    | 19       | 0.11          |
| (2,33)   | 1:104:A:ASP:H   | 1:105:A:VAL:CB   | 3        | 0.11          |
| (2,33)   | 1:104:A:ASP:H   | 1:105:A:VAL:CB   | 19       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,30)   | 1:16:A:PHE:H     | 1:17:A:GLN:CB    | 19       | 0.11          |
| (1,1250) | 1:120:A:PHE:HB2  | 1:121:A:PRO:HD2  | 10       | 0.11          |
| (1,1250) | 1:120:A:PHE:HB2  | 1:121:A:PRO:HD3  | 10       | 0.11          |
| (1,1242) | 1:130:A:TYR:H    | 1:17:A:GLN:HB2   | 11       | 0.11          |
| (1,1199) | 1:9:A:TRP:HE1    | 1:108:A:ARG:HD3  | 5        | 0.11          |
| (1,1170) | 1:52:A:SER:H     | 1:63:A:LEU:HD21  | 10       | 0.11          |
| (1,1159) | 1:127:A:PRO:HA   | 1:128:A:GLN:HG3  | 6        | 0.11          |
| (1,1159) | 1:127:A:PRO:HA   | 1:128:A:GLN:HG3  | 8        | 0.11          |
| (1,1159) | 1:127:A:PRO:HA   | 1:128:A:GLN:HG3  | 16       | 0.11          |
| (1,1159) | 1:127:A:PRO:HA   | 1:128:A:GLN:HG3  | 18       | 0.11          |
| (1,1128) | 1:73:A:GLY:HA3   | 1:102:A:PRO:HG2  | 14       | 0.11          |
| (1,1128) | 1:73:A:GLY:HA3   | 1:102:A:PRO:HG2  | 17       | 0.11          |
| (1,1013) | 1:64:A:LEU:H     | 1:63:A:LEU:HG    | 6        | 0.11          |
| (1,1008) | 1:116:A:ILE:HA   | 1:117:A:PRO:HD2  | 19       | 0.11          |
| (1,987)  | 1:32:A:ILE:HG12  | 1:120:A:PHE:HD1  | 12       | 0.11          |
| (1,987)  | 1:32:A:ILE:HG12  | 1:120:A:PHE:HD2  | 12       | 0.11          |
| (1,924)  | 1:71:A:TYR:HD2   | 1:105:A:VAL:HG23 | 11       | 0.11          |
| (1,888)  | 1:20:A:ARG:HD2   | 1:128:A:GLN:HG3  | 18       | 0.11          |
| (1,873)  | 1:78:A:ALA:H     | 1:76:A:PRO:HD3   | 4        | 0.11          |
| (1,873)  | 1:78:A:ALA:H     | 1:76:A:PRO:HD3   | 6        | 0.11          |
| (1,854)  | 1:25:A:SER:H     | 1:29:A:GLY:H     | 2        | 0.11          |
| (1,854)  | 1:25:A:SER:H     | 1:29:A:GLY:H     | 11       | 0.11          |
| (1,808)  | 1:116:A:ILE:HG23 | 1:117:A:PRO:HD3  | 8        | 0.11          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 2        | 0.11          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 5        | 0.11          |
| (1,711)  | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 18       | 0.11          |
| (1,706)  | 1:61:A:LYS:H     | 1:60:A:GLN:HB2   | 17       | 0.11          |
| (1,705)  | 1:73:A:GLY:HA3   | 1:102:A:PRO:HB2  | 2        | 0.11          |
| (1,705)  | 1:73:A:GLY:HA3   | 1:102:A:PRO:HB2  | 7        | 0.11          |
| (1,702)  | 1:58:A:GLY:H     | 1:57:A:ASP:HB3   | 1        | 0.11          |
| (1,702)  | 1:58:A:GLY:H     | 1:57:A:ASP:HB3   | 4        | 0.11          |
| (1,695)  | 1:52:A:SER:H     | 1:63:A:LEU:HD21  | 10       | 0.11          |
| (1,680)  | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 7        | 0.11          |
| (1,680)  | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 13       | 0.11          |
| (1,676)  | 1:117:A:PRO:HA   | 1:135:A:SER:HA   | 5        | 0.11          |
| (1,648)  | 1:15:A:GLN:H     | 1:13:A:ILE:HG23  | 6        | 0.11          |
| (1,626)  | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 1        | 0.11          |
| (1,626)  | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 3        | 0.11          |
| (1,626)  | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 4        | 0.11          |
| (1,626)  | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 8        | 0.11          |
| (1,626)  | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 10       | 0.11          |
| (1,626)  | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 11       | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21 | 12       | 0.11          |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21 | 14       | 0.11          |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21 | 16       | 0.11          |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21 | 19       | 0.11          |
| (1,620) | 1:89:A:VAL:HG12  | 1:86:A:LEU:HB3  | 2        | 0.11          |
| (1,620) | 1:89:A:VAL:HG11  | 1:86:A:LEU:HB3  | 2        | 0.11          |
| (1,620) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HB3  | 2        | 0.11          |
| (1,599) | 1:84:A:GLU:HB2   | 1:86:A:LEU:HD22 | 11       | 0.11          |
| (1,595) | 1:115:A:ALA:HA   | 1:114:A:GLU:HB2 | 5        | 0.11          |
| (1,550) | 1:100:A:SER:H    | 1:99:A:THR:H    | 1        | 0.11          |
| (1,509) | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 2        | 0.11          |
| (1,509) | 1:44:A:TYR:H     | 1:72:A:LEU:H    | 9        | 0.11          |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG12 | 14       | 0.11          |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG11 | 14       | 0.11          |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG13 | 14       | 0.11          |
| (1,471) | 1:84:A:GLU:H     | 1:86:A:LEU:HD23 | 6        | 0.11          |
| (1,385) | 1:118:A:THR:H    | 1:117:A:PRO:HB2 | 6        | 0.11          |
| (1,384) | 1:31:A:PRO:HB3   | 1:10:A:PHE:HE1  | 8        | 0.11          |
| (1,384) | 1:31:A:PRO:HB3   | 1:10:A:PHE:HE2  | 8        | 0.11          |
| (1,383) | 1:129:A:GLY:H    | 1:128:A:GLN:HG3 | 5        | 0.11          |
| (1,351) | 1:130:A:TYR:H    | 1:129:A:GLY:HA2 | 5        | 0.11          |
| (1,351) | 1:130:A:TYR:H    | 1:129:A:GLY:HA2 | 8        | 0.11          |
| (1,343) | 1:97:A:ALA:H     | 1:39:A:SER:HA   | 11       | 0.11          |
| (1,315) | 1:74:A:THR:H     | 1:73:A:GLY:HA2  | 4        | 0.11          |
| (1,302) | 1:43:A:GLY:HA3   | 1:72:A:LEU:H    | 15       | 0.11          |
| (1,301) | 1:43:A:GLY:HA3   | 1:71:A:TYR:H    | 17       | 0.11          |
| (1,295) | 1:10:A:PHE:H     | 1:9:A:TRP:HB3   | 17       | 0.11          |
| (1,295) | 1:10:A:PHE:H     | 1:9:A:TRP:HB2   | 17       | 0.11          |
| (1,288) | 1:16:A:PHE:HA    | 1:64:A:LEU:HD23 | 6        | 0.11          |
| (1,288) | 1:16:A:PHE:HA    | 1:64:A:LEU:HD23 | 9        | 0.11          |
| (1,288) | 1:16:A:PHE:HA    | 1:64:A:LEU:HD23 | 11       | 0.11          |
| (1,276) | 1:112:A:THR:H    | 1:109:A:ASP:H   | 19       | 0.11          |
| (1,257) | 1:116:A:ILE:HG23 | 1:10:A:PHE:HA   | 2        | 0.11          |
| (1,223) | 1:24:A:PHE:H     | 1:23:A:LYS:HB3  | 18       | 0.11          |
| (1,190) | 1:28:A:GLN:H     | 1:24:A:PHE:HB3  | 13       | 0.11          |
| (1,163) | 1:128:A:GLN:H    | 1:127:A:PRO:HA  | 19       | 0.11          |
| (1,159) | 1:126:A:LEU:H    | 1:125:A:ILE:HA  | 7        | 0.11          |
| (1,123) | 1:22:A:PHE:H     | 1:21:A:ASP:HA   | 3        | 0.11          |
| (1,95)  | 1:34:A:PHE:HD2   | 1:71:A:TYR:HE1  | 8        | 0.11          |
| (1,83)  | 1:46:A:TYR:HD1   | 1:76:A:PRO:HD3  | 12       | 0.11          |
| (1,83)  | 1:46:A:TYR:HD2   | 1:76:A:PRO:HD3  | 12       | 0.11          |
| (1,81)  | 1:13:A:ILE:HA    | 1:133:A:GLU:H   | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,81)   | 1:13:A:ILE:HA   | 1:133:A:GLU:H    | 17       | 0.11          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3   | 10       | 0.11          |
| (1,47)   | 1:25:A:SER:HA   | 1:28:A:GLN:HB3   | 19       | 0.11          |
| (1,7)    | 1:48:A:HIS:HB3  | 1:68:A:TYR:HE1   | 5        | 0.11          |
| (1,7)    | 1:48:A:HIS:HB3  | 1:68:A:TYR:HE2   | 5        | 0.11          |
| (1,6)    | 1:44:A:TYR:H    | 1:91:A:TRP:HZ3   | 2        | 0.11          |
| (1,6)    | 1:44:A:TYR:H    | 1:91:A:TRP:HZ3   | 3        | 0.11          |
| (2,1201) | 1:52:A:SER:CB   | 1:62:A:GLN:CB    | 16       | 0.1           |
| (2,1091) | 1:103:A:SER:H   | 1:72:A:LEU:H     | 11       | 0.1           |
| (2,945)  | 1:22:A:PHE:CA   | 1:127:A:PRO:CB   | 10       | 0.1           |
| (2,885)  | 1:32:A:ILE:CB   | 1:120:A:PHE:CB   | 12       | 0.1           |
| (2,853)  | 1:6:A:HIS:CB    | 1:4:A:ILE:CB     | 18       | 0.1           |
| (2,777)  | 1:25:A:SER:H    | 1:29:A:GLY:H     | 1        | 0.1           |
| (2,777)  | 1:25:A:SER:H    | 1:29:A:GLY:H     | 4        | 0.1           |
| (2,754)  | 1:101:A:THR:H   | 1:98:A:ASP:H     | 3        | 0.1           |
| (2,754)  | 1:101:A:THR:H   | 1:98:A:ASP:H     | 8        | 0.1           |
| (2,699)  | 1:111:A:THR:CB  | 1:110:A:PRO:CB   | 8        | 0.1           |
| (2,643)  | 1:68:A:TYR:H    | 1:48:A:HIS:H     | 2        | 0.1           |
| (2,538)  | 1:13:A:ILE:H    | 1:69:A:PHE:CB    | 6        | 0.1           |
| (2,469)  | 1:44:A:TYR:H    | 1:72:A:LEU:H     | 1        | 0.1           |
| (2,451)  | 1:43:A:GLY:H    | 1:92:A:VAL:H     | 6        | 0.1           |
| (2,444)  | 1:104:A:ASP:CB  | 1:36:A:VAL:CB    | 10       | 0.1           |
| (2,431)  | 1:120:A:PHE:H   | 1:32:A:ILE:CB    | 1        | 0.1           |
| (2,369)  | 1:96:A:GLN:CB   | 1:38:A:PRO:CB    | 8        | 0.1           |
| (2,361)  | 1:81:A:SER:H    | 1:84:A:GLU:CB    | 9        | 0.1           |
| (2,261)  | 1:108:A:ARG:H   | 1:107:A:SER:H    | 16       | 0.1           |
| (2,233)  | 1:39:A:SER:H    | 1:40:A:GLU:H     | 6        | 0.1           |
| (1,1241) | 1:130:A:TYR:H   | 1:127:A:PRO:HB3  | 16       | 0.1           |
| (1,1228) | 1:103:A:SER:H   | 1:72:A:LEU:H     | 11       | 0.1           |
| (1,1211) | 1:43:A:GLY:H    | 1:72:A:LEU:HB3   | 15       | 0.1           |
| (1,1159) | 1:127:A:PRO:HA  | 1:128:A:GLN:HG3  | 2        | 0.1           |
| (1,1159) | 1:127:A:PRO:HA  | 1:128:A:GLN:HG3  | 14       | 0.1           |
| (1,1159) | 1:127:A:PRO:HA  | 1:128:A:GLN:HG3  | 15       | 0.1           |
| (1,1156) | 1:63:A:LEU:HA   | 1:62:A:GLN:HB2   | 15       | 0.1           |
| (1,1120) | 1:130:A:TYR:H   | 1:13:A:ILE:HG23  | 12       | 0.1           |
| (1,1013) | 1:64:A:LEU:H    | 1:63:A:LEU:HG    | 9        | 0.1           |
| (1,927)  | 1:71:A:TYR:HE2  | 1:105:A:VAL:HG23 | 19       | 0.1           |
| (1,874)  | 1:126:A:LEU:HB2 | 1:127:A:PRO:HD3  | 5        | 0.1           |
| (1,854)  | 1:25:A:SER:H    | 1:29:A:GLY:H     | 1        | 0.1           |
| (1,854)  | 1:25:A:SER:H    | 1:29:A:GLY:H     | 4        | 0.1           |
| (1,829)  | 1:101:A:THR:H   | 1:98:A:ASP:H     | 3        | 0.1           |
| (1,829)  | 1:101:A:THR:H   | 1:98:A:ASP:H     | 8        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,802) | 1:43:A:GLY:HA2   | 1:71:A:TYR:H     | 17       | 0.1           |
| (1,745) | 1:91:A:TRP:H     | 1:90:A:PHE:HB3   | 15       | 0.1           |
| (1,712) | 1:68:A:TYR:H     | 1:48:A:HIS:H     | 2        | 0.1           |
| (1,711) | 1:47:A:ARG:HA    | 1:67:A:TRP:HE1   | 6        | 0.1           |
| (1,680) | 1:41:A:ALA:H     | 1:36:A:VAL:HG23  | 1        | 0.1           |
| (1,653) | 1:16:A:PHE:H     | 1:64:A:LEU:HD21  | 13       | 0.1           |
| (1,648) | 1:15:A:GLN:H     | 1:13:A:ILE:HG23  | 3        | 0.1           |
| (1,641) | 1:108:A:ARG:HB3  | 1:9:A:TRP:HE1    | 13       | 0.1           |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 7        | 0.1           |
| (1,626) | 1:89:A:VAL:HG13  | 1:86:A:LEU:HD21  | 13       | 0.1           |
| (1,509) | 1:44:A:TYR:H     | 1:72:A:LEU:H     | 1        | 0.1           |
| (1,491) | 1:43:A:GLY:H     | 1:92:A:VAL:H     | 6        | 0.1           |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG12  | 5        | 0.1           |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG11  | 5        | 0.1           |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG13  | 5        | 0.1           |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG12  | 12       | 0.1           |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG11  | 12       | 0.1           |
| (1,473) | 1:86:A:LEU:H     | 1:89:A:VAL:HG13  | 12       | 0.1           |
| (1,416) | 1:97:A:ALA:H     | 1:96:A:GLN:HB3   | 4        | 0.1           |
| (1,351) | 1:130:A:TYR:H    | 1:129:A:GLY:HA2  | 1        | 0.1           |
| (1,351) | 1:130:A:TYR:H    | 1:129:A:GLY:HA2  | 9        | 0.1           |
| (1,347) | 1:89:A:VAL:H     | 1:88:A:GLY:HA3   | 4        | 0.1           |
| (1,347) | 1:89:A:VAL:H     | 1:88:A:GLY:HA3   | 10       | 0.1           |
| (1,315) | 1:74:A:THR:H     | 1:73:A:GLY:HA2   | 1        | 0.1           |
| (1,315) | 1:74:A:THR:H     | 1:73:A:GLY:HA2   | 11       | 0.1           |
| (1,288) | 1:16:A:PHE:HA    | 1:64:A:LEU:HD23  | 8        | 0.1           |
| (1,284) | 1:108:A:ARG:H    | 1:107:A:SER:H    | 16       | 0.1           |
| (1,257) | 1:116:A:ILE:HG23 | 1:10:A:PHE:HA    | 3        | 0.1           |
| (1,252) | 1:39:A:SER:H     | 1:40:A:GLU:H     | 6        | 0.1           |
| (1,123) | 1:22:A:PHE:H     | 1:21:A:ASP:HA    | 6        | 0.1           |
| (1,120) | 1:24:A:PHE:HA    | 1:125:A:ILE:HG23 | 13       | 0.1           |
| (1,120) | 1:24:A:PHE:HA    | 1:125:A:ILE:HG23 | 15       | 0.1           |
| (1,95)  | 1:34:A:PHE:HD2   | 1:71:A:TYR:HE1   | 1        | 0.1           |
| (1,54)  | 1:63:A:LEU:HA    | 1:62:A:GLN:HG2   | 5        | 0.1           |
| (1,19)  | 1:77:A:TYR:H     | 1:76:A:PRO:HG3   | 6        | 0.1           |
| (1,19)  | 1:77:A:TYR:H     | 1:76:A:PRO:HG3   | 16       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found