



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 06:42 PM EST

PDB ID : 2LX0
BMRB ID : 18655
Title : Arced helix (ArcH) NMR structure of the reovirus p14 fusion-associated small transmembrane (FAST) protein transmembrane domain (TMD) in dodecyl phosphocholine (DPC) micelles
Authors : Sarker, M.; Key, T.; Duncan, R.; Rainey, J.K.
Deposited on : 2012-08-10

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

We welcome your comments at validation@mail.wwpdb.org

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>.

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

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

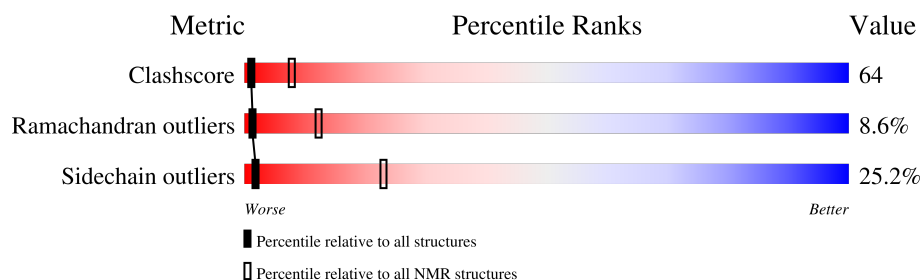
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 57%.

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 (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 210492 | 14027 |
| Ramachandran outliers | 207382 | 12486 |
| Sidechain outliers | 206894 | 12463 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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 | 32 | |

2 Ensemble composition and analysis

This entry contains 50 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:4-A:31 (28) | 0.38 | 10 |

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 7 clusters and 4 single-model clusters were found.

| Cluster number | Models |
|-----------------------|--|
| 1 | 1, 2, 3, 6, 10, 11, 13, 20, 22, 23, 25, 28, 32, 33, 34, 36, 37, 40, 47 |
| 2 | 4, 9, 15, 21, 24, 27, 38, 43, 44 |
| 3 | 5, 7, 8, 12, 14, 17, 39, 50 |
| 4 | 19, 29, 30, 31 |
| 5 | 35, 41 |
| 6 | 16, 18 |
| 7 | 42, 48 |
| Single-model clusters | 26; 45; 46; 49 |

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 567 atoms, of which 294 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Membrane fusion protein p14.

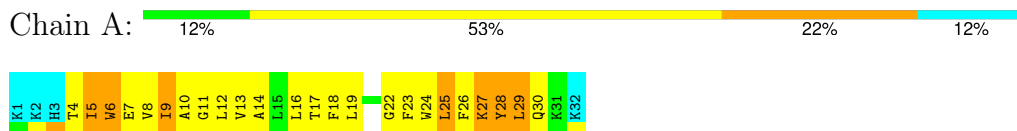
| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1 | A | 32 | Total | C | H | N | O | 0 |
| | | | 567 | 192 | 294 | 42 | 39 | |

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: Membrane fusion protein p14

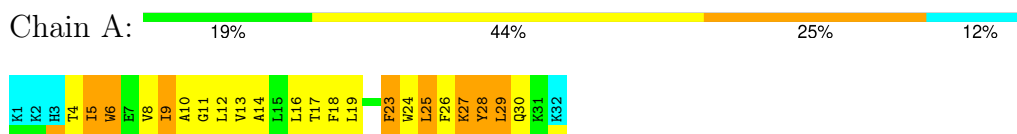


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

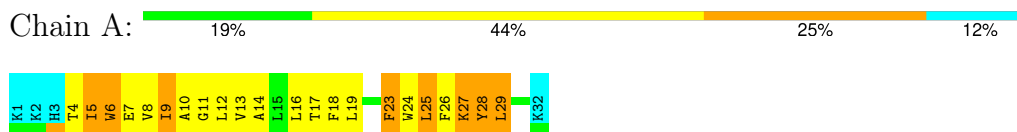
4.2.1 Score per residue for model 1

- Molecule 1: Membrane fusion protein p14



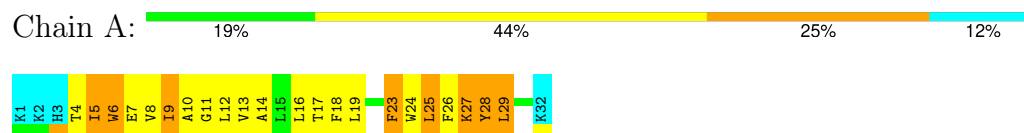
4.2.2 Score per residue for model 2

- Molecule 1: Membrane fusion protein p14



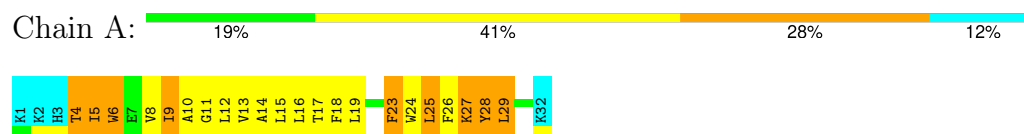
4.2.3 Score per residue for model 3

- Molecule 1: Membrane fusion protein p14



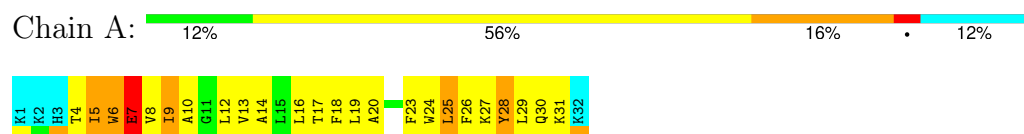
4.2.4 Score per residue for model 4

- Molecule 1: Membrane fusion protein p14



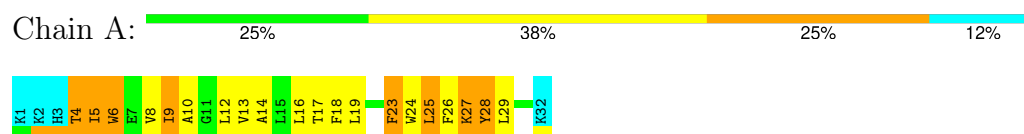
4.2.5 Score per residue for model 5

- Molecule 1: Membrane fusion protein p14



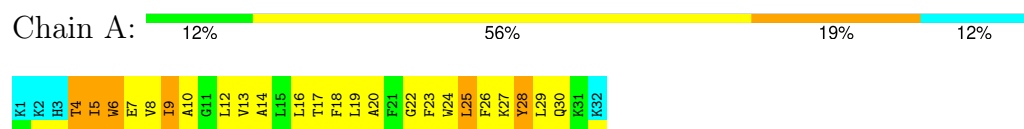
4.2.6 Score per residue for model 6

- Molecule 1: Membrane fusion protein p14



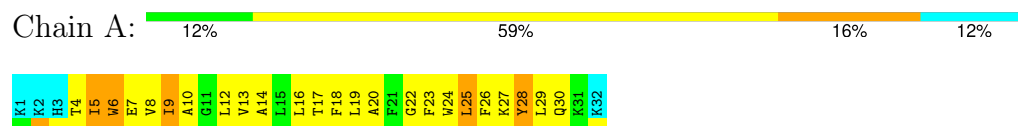
4.2.7 Score per residue for model 7

- Molecule 1: Membrane fusion protein p14



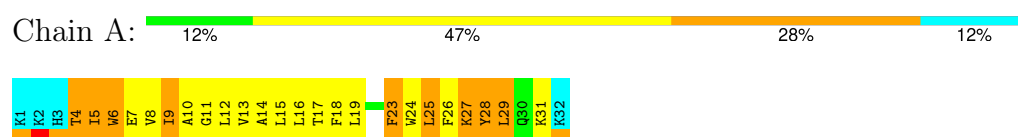
4.2.8 Score per residue for model 8

- Molecule 1: Membrane fusion protein p14



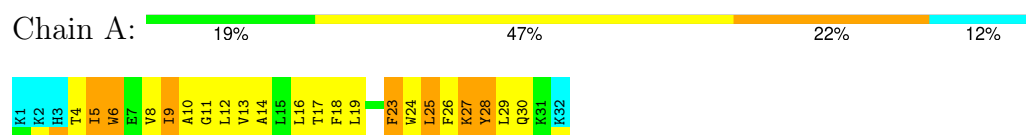
4.2.9 Score per residue for model 9

- Molecule 1: Membrane fusion protein p14



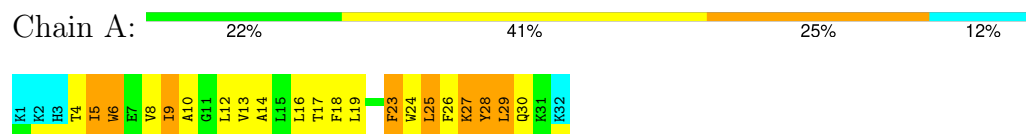
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Membrane fusion protein p14



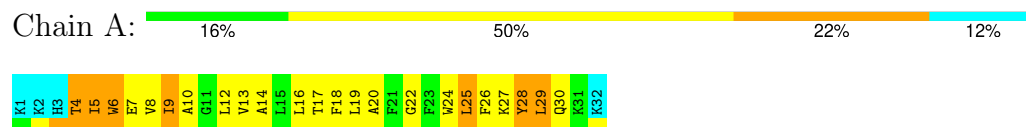
4.2.11 Score per residue for model 11

- Molecule 1: Membrane fusion protein p14



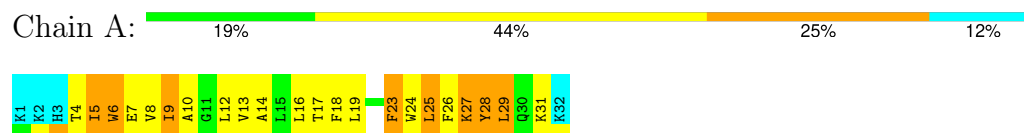
4.2.12 Score per residue for model 12

- Molecule 1: Membrane fusion protein p14



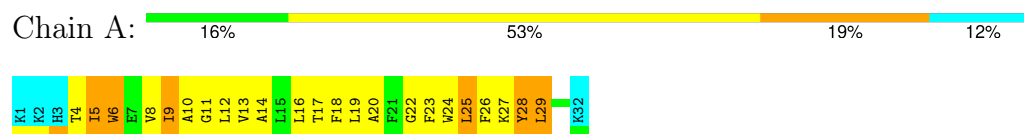
4.2.13 Score per residue for model 13

- Molecule 1: Membrane fusion protein p14



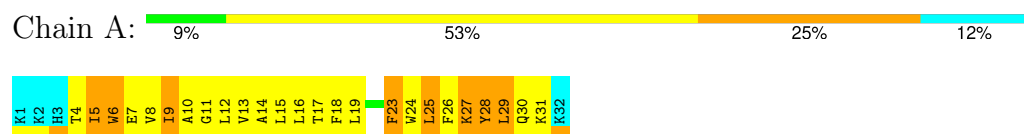
4.2.14 Score per residue for model 14

- Molecule 1: Membrane fusion protein p14



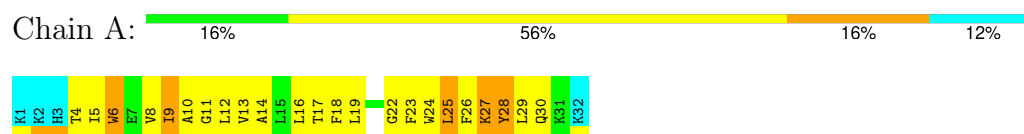
4.2.15 Score per residue for model 15

- Molecule 1: Membrane fusion protein p14



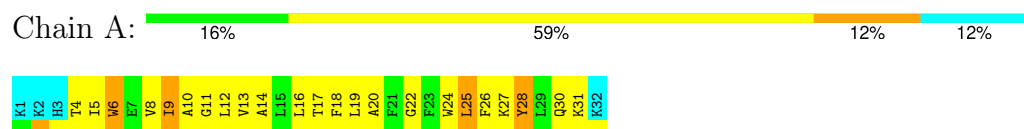
4.2.16 Score per residue for model 16

- Molecule 1: Membrane fusion protein p14



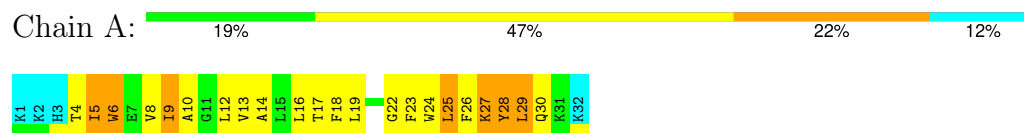
4.2.17 Score per residue for model 17

- Molecule 1: Membrane fusion protein p14



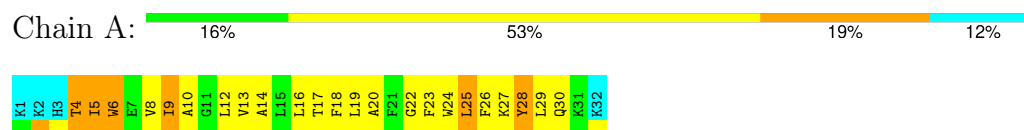
4.2.18 Score per residue for model 18

- Molecule 1: Membrane fusion protein p14



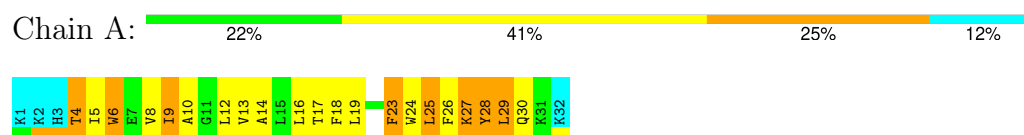
4.2.19 Score per residue for model 19

- Molecule 1: Membrane fusion protein p14



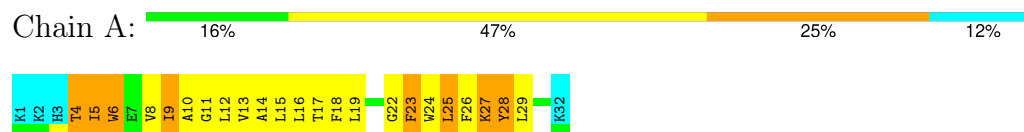
4.2.20 Score per residue for model 20

- Molecule 1: Membrane fusion protein p14



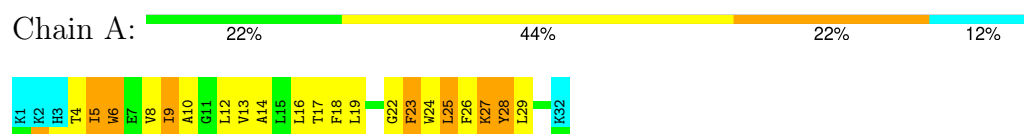
4.2.21 Score per residue for model 21

- Molecule 1: Membrane fusion protein p14



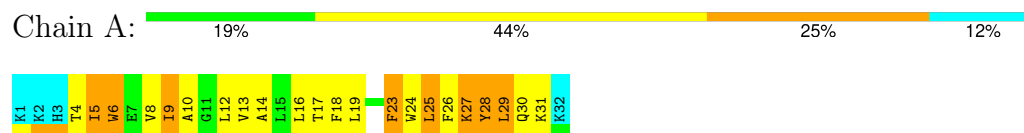
4.2.22 Score per residue for model 22

- Molecule 1: Membrane fusion protein p14



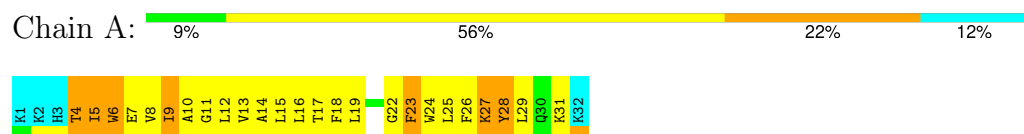
4.2.23 Score per residue for model 23

- Molecule 1: Membrane fusion protein p14



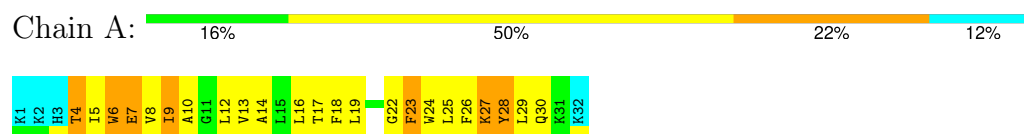
4.2.24 Score per residue for model 24

- Molecule 1: Membrane fusion protein p14



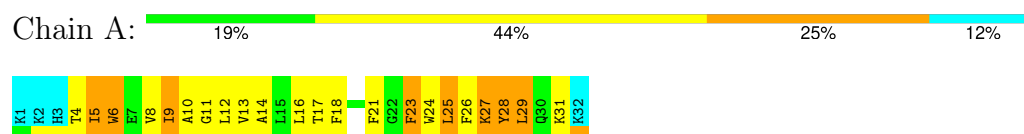
4.2.25 Score per residue for model 25

- Molecule 1: Membrane fusion protein p14



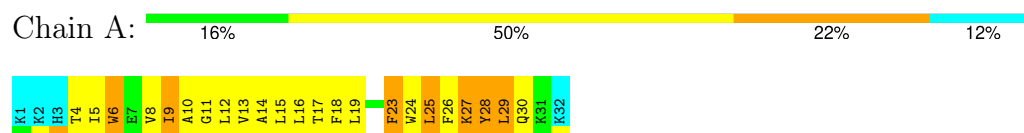
4.2.26 Score per residue for model 26

- Molecule 1: Membrane fusion protein p14



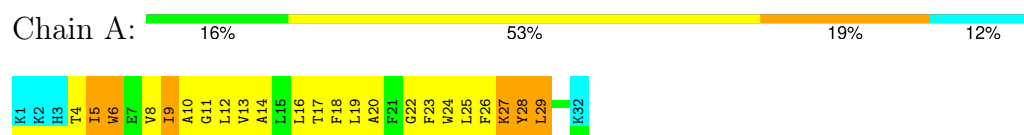
4.2.27 Score per residue for model 27

- Molecule 1: Membrane fusion protein p14



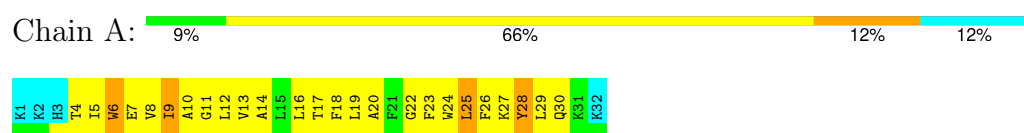
4.2.28 Score per residue for model 28

- Molecule 1: Membrane fusion protein p14



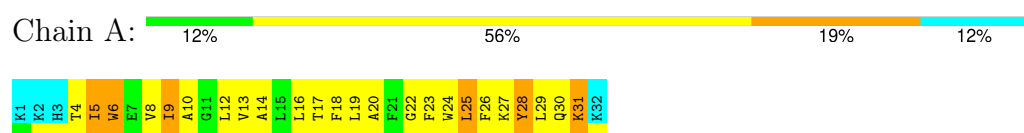
4.2.29 Score per residue for model 29

- Molecule 1: Membrane fusion protein p14



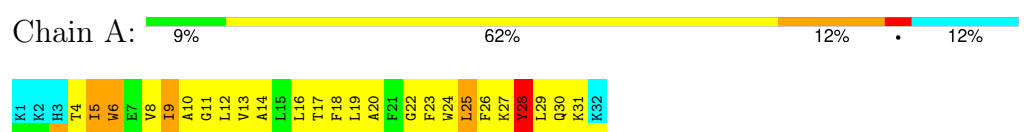
4.2.30 Score per residue for model 30

- Molecule 1: Membrane fusion protein p14



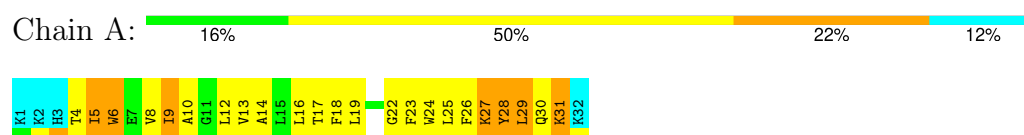
4.2.31 Score per residue for model 31

- Molecule 1: Membrane fusion protein p14



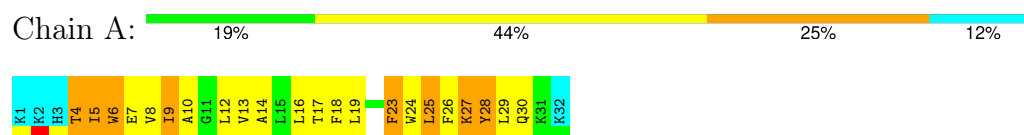
4.2.32 Score per residue for model 32

- Molecule 1: Membrane fusion protein p14



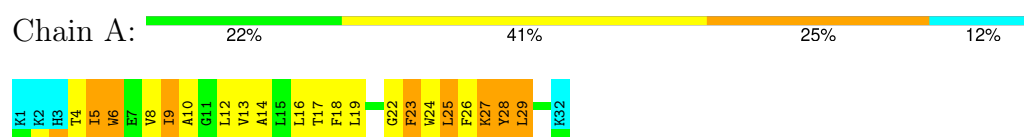
4.2.33 Score per residue for model 33

- Molecule 1: Membrane fusion protein p14



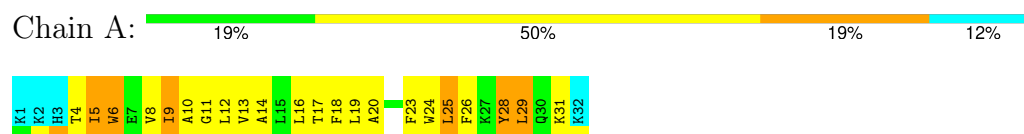
4.2.34 Score per residue for model 34

- Molecule 1: Membrane fusion protein p14



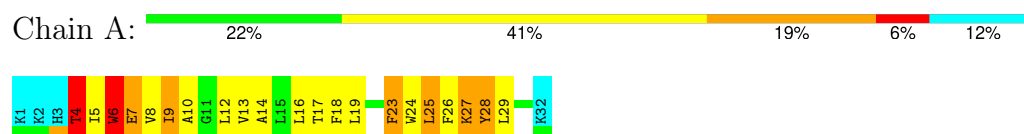
4.2.35 Score per residue for model 35

- Molecule 1: Membrane fusion protein p14



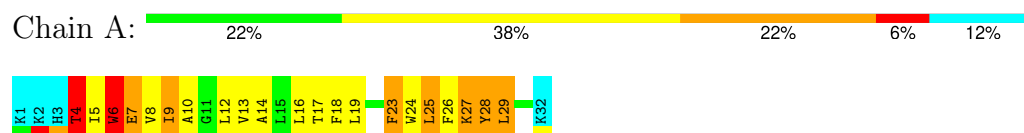
4.2.36 Score per residue for model 36

- Molecule 1: Membrane fusion protein p14



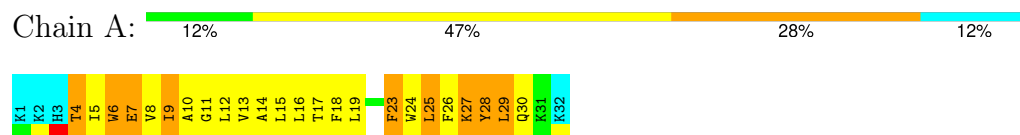
4.2.37 Score per residue for model 37

- Molecule 1: Membrane fusion protein p14



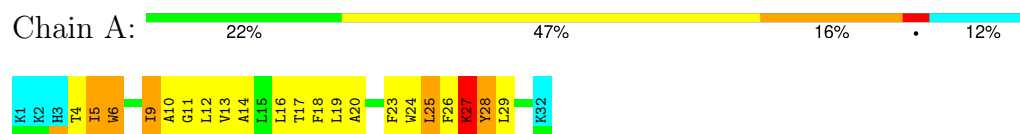
4.2.38 Score per residue for model 38

- Molecule 1: Membrane fusion protein p14



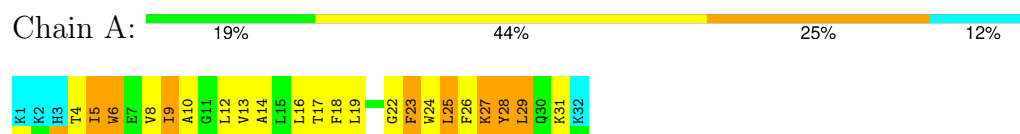
4.2.39 Score per residue for model 39

- Molecule 1: Membrane fusion protein p14



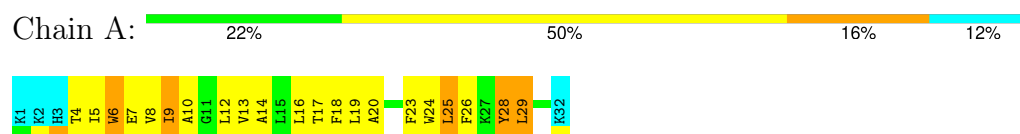
4.2.40 Score per residue for model 40

- Molecule 1: Membrane fusion protein p14



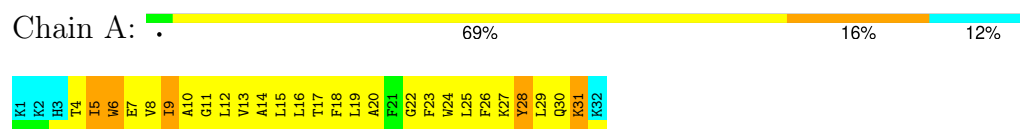
4.2.41 Score per residue for model 41

- Molecule 1: Membrane fusion protein p14



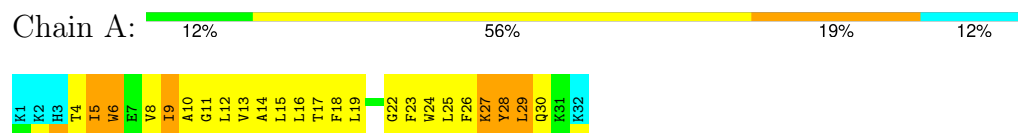
4.2.42 Score per residue for model 42

- Molecule 1: Membrane fusion protein p14



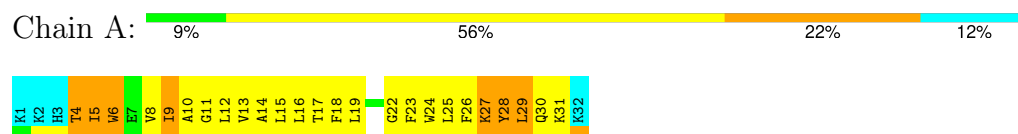
4.2.43 Score per residue for model 43

- Molecule 1: Membrane fusion protein p14



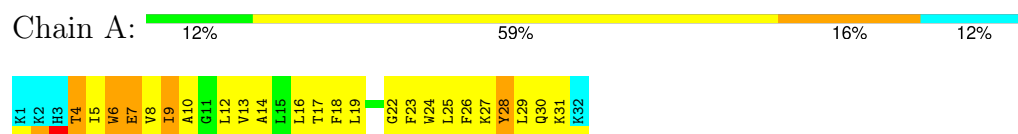
4.2.44 Score per residue for model 44

- Molecule 1: Membrane fusion protein p14



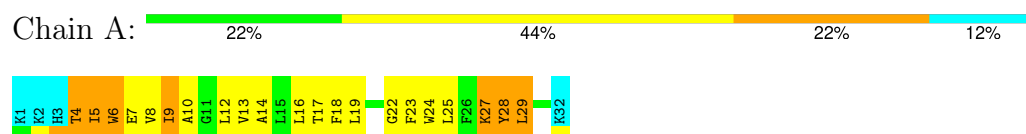
4.2.45 Score per residue for model 45

- Molecule 1: Membrane fusion protein p14



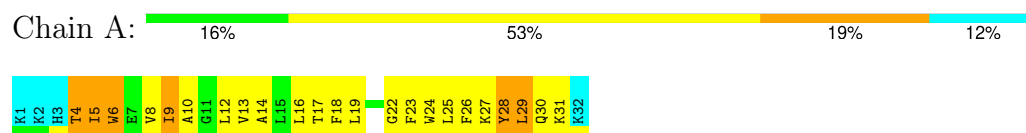
4.2.46 Score per residue for model 46

- Molecule 1: Membrane fusion protein p14



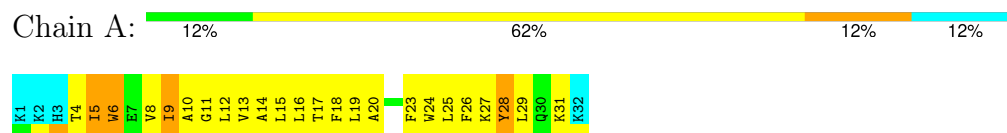
4.2.47 Score per residue for model 47

- Molecule 1: Membrane fusion protein p14



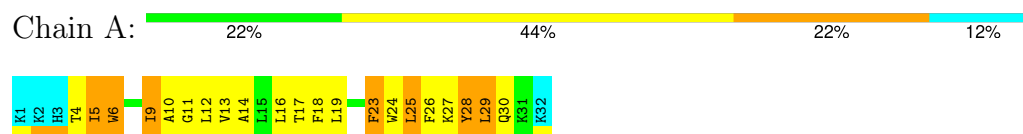
4.2.48 Score per residue for model 48

- Molecule 1: Membrane fusion protein p14



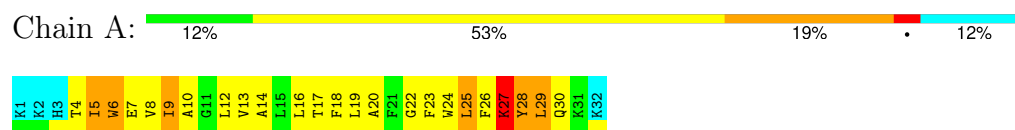
4.2.49 Score per residue for model 49

- Molecule 1: Membrane fusion protein p14



4.2.50 Score per residue for model 50

- Molecule 1: Membrane fusion protein p14



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 50 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 |
|---------------|--------------------|---------|
| X-PLOR NIH | structure solution | 2.18 |
| X-PLOR NIH | refinement | 2.18 |

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 | 287 |
| Number of shifts mapped to atoms | 286 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 1 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 57% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 235 | 246 | 246 | 31±3 |
| All | All | 11750 | 12300 | 12300 | 1550 |

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 64.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:11:GLY:O | 1:A:15:LEU:HD12 | 0.67 | 1.90 | 42 | 11 |
| 1:A:29:LEU:HD12 | 1:A:29:LEU:O | 0.64 | 1.92 | 43 | 2 |
| 1:A:24:TRP:CZ2 | 1:A:28:TYR:CD2 | 0.62 | 2.88 | 46 | 20 |
| 1:A:24:TRP:CZ2 | 1:A:28:TYR:CE2 | 0.62 | 2.87 | 12 | 16 |
| 1:A:4:THR:HG23 | 1:A:5:ILE:N | 0.61 | 2.09 | 19 | 46 |
| 1:A:29:LEU:C | 1:A:29:LEU:HD12 | 0.60 | 2.17 | 47 | 1 |
| 1:A:29:LEU:HD12 | 1:A:29:LEU:C | 0.60 | 2.17 | 43 | 1 |
| 1:A:24:TRP:CE2 | 1:A:28:TYR:CD2 | 0.59 | 2.90 | 14 | 19 |
| 1:A:6:TRP:O | 1:A:10:ALA:N | 0.58 | 2.36 | 20 | 50 |
| 1:A:4:THR:HG23 | 1:A:5:ILE:H | 0.58 | 1.59 | 11 | 44 |
| 1:A:29:LEU:O | 1:A:29:LEU:HD23 | 0.57 | 2.00 | 7 | 25 |
| 1:A:26:PHE:O | 1:A:30:GLN:N | 0.56 | 2.38 | 49 | 17 |
| 1:A:22:GLY:O | 1:A:26:PHE:CD2 | 0.55 | 2.60 | 16 | 17 |
| 1:A:10:ALA:O | 1:A:14:ALA:N | 0.54 | 2.40 | 49 | 50 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:14:ALA:O | 1:A:18:PHE:N | 0.54 | 2.40 | 40 | 50 |
| 1:A:13:VAL:O | 1:A:16:LEU:N | 0.54 | 2.40 | 49 | 50 |
| 1:A:4:THR:OG1 | 1:A:5:ILE:N | 0.54 | 2.41 | 38 | 50 |
| 1:A:19:LEU:HD22 | 1:A:19:LEU:N | 0.54 | 2.17 | 39 | 6 |
| 1:A:4:THR:HG23 | 1:A:6:TRP:H | 0.54 | 1.62 | 19 | 13 |
| 1:A:13:VAL:O | 1:A:17:THR:N | 0.54 | 2.41 | 14 | 50 |
| 1:A:19:LEU:N | 1:A:19:LEU:CD2 | 0.54 | 2.71 | 46 | 48 |
| 1:A:19:LEU:N | 1:A:19:LEU:HD22 | 0.53 | 2.19 | 46 | 42 |
| 1:A:9:ILE:O | 1:A:13:VAL:N | 0.53 | 2.42 | 37 | 50 |
| 1:A:26:PHE:O | 1:A:28:TYR:N | 0.53 | 2.42 | 44 | 41 |
| 1:A:23:PHE:CG | 1:A:23:PHE:O | 0.52 | 2.62 | 35 | 4 |
| 1:A:23:PHE:O | 1:A:23:PHE:CG | 0.52 | 2.63 | 46 | 3 |
| 1:A:9:ILE:O | 1:A:13:VAL:HG23 | 0.52 | 2.04 | 27 | 41 |
| 1:A:24:TRP:O | 1:A:27:LYS:N | 0.51 | 2.42 | 46 | 1 |
| 1:A:6:TRP:O | 1:A:8:VAL:N | 0.51 | 2.43 | 25 | 21 |
| 1:A:10:ALA:C | 1:A:12:LEU:N | 0.51 | 2.64 | 27 | 50 |
| 1:A:26:PHE:C | 1:A:28:TYR:H | 0.51 | 2.08 | 16 | 44 |
| 1:A:10:ALA:O | 1:A:13:VAL:N | 0.50 | 2.45 | 41 | 50 |
| 1:A:17:THR:O | 1:A:20:ALA:N | 0.50 | 2.44 | 12 | 17 |
| 1:A:5:ILE:O | 1:A:8:VAL:N | 0.50 | 2.44 | 24 | 46 |
| 1:A:24:TRP:O | 1:A:25:LEU:C | 0.50 | 2.50 | 33 | 50 |
| 1:A:19:LEU:CD1 | 1:A:19:LEU:N | 0.50 | 2.74 | 40 | 1 |
| 1:A:4:THR:CG2 | 1:A:5:ILE:N | 0.50 | 2.74 | 19 | 21 |
| 1:A:27:LYS:CD | 1:A:27:LYS:N | 0.50 | 2.75 | 18 | 6 |
| 1:A:28:TYR:CD1 | 1:A:28:TYR:C | 0.49 | 2.85 | 47 | 31 |
| 1:A:30:GLN:CG | 1:A:30:GLN:O | 0.49 | 2.60 | 32 | 9 |
| 1:A:29:LEU:O | 1:A:29:LEU:HD13 | 0.49 | 2.08 | 40 | 2 |
| 1:A:24:TRP:NE1 | 1:A:28:TYR:CG | 0.48 | 2.81 | 17 | 1 |
| 1:A:4:THR:CG2 | 1:A:5:ILE:H | 0.48 | 2.20 | 29 | 42 |
| 1:A:19:LEU:N | 1:A:19:LEU:HD12 | 0.48 | 2.24 | 40 | 1 |
| 1:A:6:TRP:C | 1:A:8:VAL:N | 0.48 | 2.67 | 25 | 26 |
| 1:A:12:LEU:O | 1:A:16:LEU:CD1 | 0.48 | 2.62 | 26 | 46 |
| 1:A:23:PHE:O | 1:A:27:LYS:CG | 0.48 | 2.62 | 15 | 26 |
| 1:A:26:PHE:C | 1:A:28:TYR:N | 0.47 | 2.68 | 23 | 39 |
| 1:A:6:TRP:O | 1:A:11:GLY:N | 0.47 | 2.47 | 27 | 19 |
| 1:A:12:LEU:O | 1:A:16:LEU:HD12 | 0.47 | 2.09 | 17 | 33 |
| 1:A:28:TYR:C | 1:A:28:TYR:CD1 | 0.47 | 2.84 | 43 | 1 |
| 1:A:25:LEU:O | 1:A:29:LEU:N | 0.47 | 2.43 | 34 | 4 |
| 1:A:28:TYR:CG | 1:A:29:LEU:N | 0.46 | 2.83 | 46 | 10 |
| 1:A:29:LEU:C | 1:A:29:LEU:CD1 | 0.46 | 2.83 | 47 | 2 |
| 1:A:7:GLU:N | 1:A:7:GLU:OE1 | 0.45 | 2.50 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:26:PHE:O | 1:A:30:GLN:CB | 0.45 | 2.64 | 49 | 1 |
| 1:A:28:TYR:O | 1:A:28:TYR:CD1 | 0.45 | 2.70 | 21 | 4 |
| 1:A:10:ALA:O | 1:A:12:LEU:N | 0.44 | 2.51 | 27 | 50 |
| 1:A:6:TRP:CG | 1:A:10:ALA:CB | 0.44 | 3.00 | 4 | 43 |
| 1:A:30:GLN:O | 1:A:30:GLN:CG | 0.44 | 2.65 | 16 | 4 |
| 1:A:24:TRP:O | 1:A:28:TYR:N | 0.44 | 2.49 | 49 | 1 |
| 1:A:25:LEU:O | 1:A:29:LEU:CB | 0.44 | 2.66 | 33 | 10 |
| 1:A:22:GLY:C | 1:A:24:TRP:N | 0.43 | 2.69 | 40 | 7 |
| 1:A:18:PHE:O | 1:A:22:GLY:N | 0.43 | 2.47 | 25 | 6 |
| 1:A:24:TRP:NE1 | 1:A:28:TYR:CB | 0.43 | 2.82 | 17 | 1 |
| 1:A:10:ALA:C | 1:A:12:LEU:H | 0.42 | 2.18 | 49 | 36 |
| 1:A:6:TRP:C | 1:A:8:VAL:H | 0.42 | 2.17 | 29 | 8 |
| 1:A:27:LYS:CD | 1:A:27:LYS:H | 0.42 | 2.25 | 50 | 1 |
| 1:A:5:ILE:O | 1:A:6:TRP:C | 0.42 | 2.58 | 37 | 5 |
| 1:A:9:ILE:O | 1:A:13:VAL:CG2 | 0.42 | 2.68 | 27 | 1 |
| 1:A:7:GLU:N | 1:A:7:GLU:CD | 0.41 | 2.73 | 25 | 1 |
| 1:A:21:PHE:CD1 | 1:A:21:PHE:N | 0.41 | 2.89 | 26 | 1 |
| 1:A:28:TYR:CD1 | 1:A:28:TYR:O | 0.41 | 2.74 | 49 | 1 |
| 1:A:17:THR:HG22 | 1:A:18:PHE:N | 0.41 | 2.31 | 28 | 2 |

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 | 28/32 (88%) | 17±1 (62±4%) | 8±1 (29±4%) | 2±1 (9±4%) | 1 | 12 |
| All | All | 1400/1600 (88%) | 869 (62%) | 410 (29%) | 121 (9%) | 1 | 12 |

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 | 27 | LYS | 46 |
| 1 | A | 25 | LEU | 39 |
| 1 | A | 4 | THR | 18 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 7 | GLU | 15 |
| 1 | A | 6 | TRP | 2 |
| 1 | A | 28 | 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 | 23/27 (85%) | 17±1 (75±4%) | 6±1 (25±4%) | 2 | 23 |
| All | All | 1150/1350 (85%) | 860 (75%) | 290 (25%) | 2 | 23 |

All 10 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 | 6 | TRP | 50 |
| 1 | A | 9 | ILE | 50 |
| 1 | A | 28 | TYR | 50 |
| 1 | A | 23 | PHE | 41 |
| 1 | A | 5 | ILE | 39 |
| 1 | A | 29 | LEU | 36 |
| 1 | A | 31 | LYS | 12 |
| 1 | A | 7 | GLU | 7 |
| 1 | A | 27 | LYS | 3 |
| 1 | A | 4 | THR | 2 |

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 57% for the well-defined parts and 56% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

| | |
|---|-----|
| Total number of shifts | 287 |
| Number of shifts mapped to atoms | 286 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 1 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 3 | HIS | HD1 | 11.126 | 0.003 | 1 |

7.1.2 Chemical shift referencing

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

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 57%, i.e. 244 atoms were assigned a chemical shift out of a possible 427. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 66/142 (46%) | 58/58 (100%) | 0/56 (0%) | 8/28 (29%) |
| Sidechain | 142/212 (67%) | 142/143 (99%) | 0/66 (0%) | 0/3 (0%) |
| Aromatic | 36/73 (49%) | 36/36 (100%) | 0/35 (0%) | 0/2 (0%) |
| Overall | 244/427 (57%) | 236/237 (100%) | 0/157 (0%) | 8/33 (24%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 56%, i.e. 278 atoms were assigned a chemical shift out of a possible 496. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 71/162 (44%) | 63/66 (95%) | 0/64 (0%) | 8/32 (25%) |
| Sidechain | 168/254 (66%) | 168/169 (99%) | 0/79 (0%) | 0/6 (0%) |
| Aromatic | 39/80 (49%) | 39/40 (98%) | 0/37 (0%) | 0/3 (0%) |
| Overall | 278/496 (56%) | 270/275 (98%) | 0/180 (0%) | 8/41 (20%) |

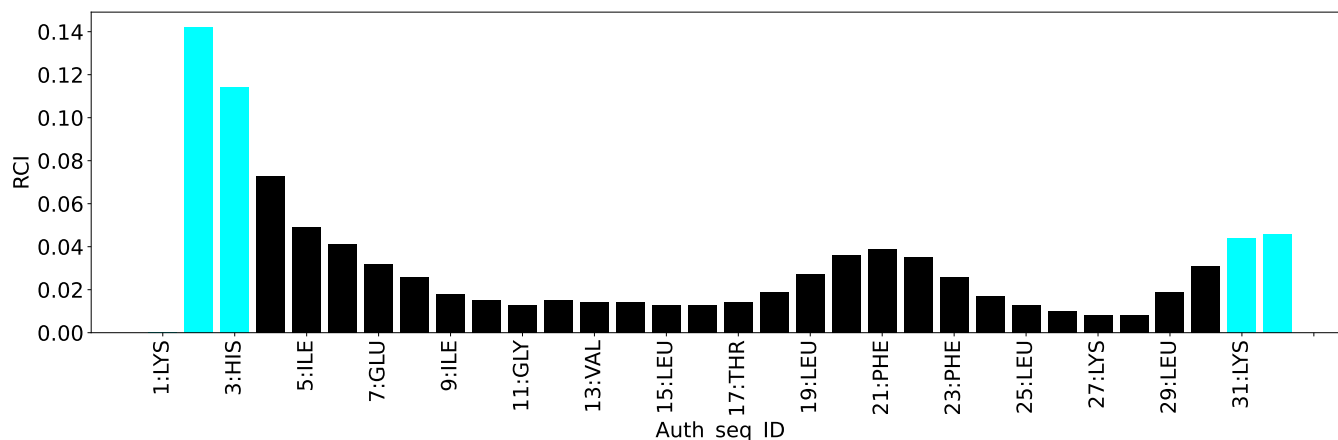
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain 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 | 1887 |
| Intra-residue ($ i-j =0$) | 739 |
| Sequential ($ i-j =1$) | 496 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 621 |
| Long range ($ i-j \geq 5$) | 11 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 20 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 38 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 60.2 |
| Number of long range restraints per residue ¹ | 0.3 |

¹Long 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) | 8.2 | 0.2 |
| 0.2-0.5 (Medium) | 11.3 | 0.5 |
| >0.5 (Large) | 8.8 | 1.62 |

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

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 1.0 | 8.84 |
| 10.0-20.0 (Medium) | 0.2 | 14.19 |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

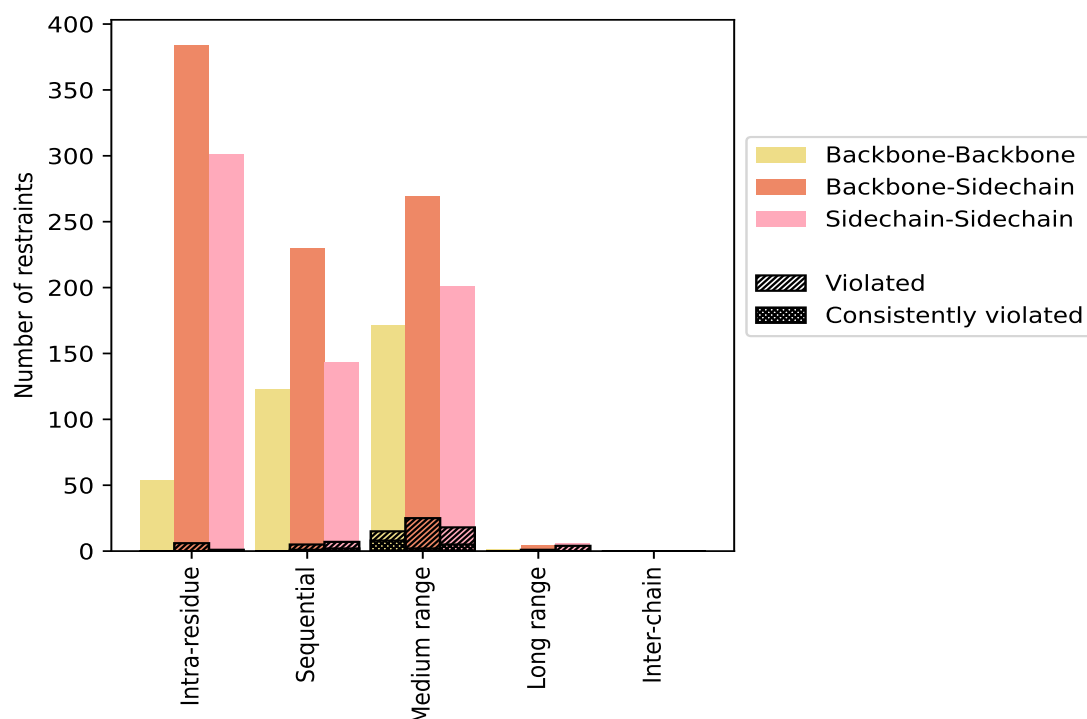
9.1 Summary of distance violations ⓘ

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|--|----------------------|-----------------------|-----------------------|----------------------|---------------------|------------------------------------|---------------------|---------------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue (i-j =0) | 739 | 39.2 | 7 | 0.9 | 0.4 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 54 | 2.9 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 384 | 20.3 | 6 | 1.6 | 0.3 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 301 | 16.0 | 1 | 0.3 | 0.1 | 0 | 0.0 | 0.0 |
| Sequential (i-j =1) | 496 | 26.3 | 12 | 2.4 | 0.6 | 3 | 0.6 | 0.2 |
| Backbone-Backbone | 123 | 6.5 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 230 | 12.2 | 5 | 2.2 | 0.3 | 1 | 0.4 | 0.1 |
| Sidechain-Sidechain | 143 | 7.6 | 7 | 4.9 | 0.4 | 2 | 1.4 | 0.1 |
| Medium range (i-j >1 & i-j <5) | 621 | 32.9 | 49 | 7.9 | 2.6 | 15 | 2.4 | 0.8 |
| Backbone-Backbone | 171 | 9.1 | 15 | 8.8 | 0.8 | 8 | 4.7 | 0.4 |
| Backbone-Sidechain | 249 | 13.2 | 16 | 6.4 | 0.8 | 2 | 0.8 | 0.1 |
| Sidechain-Sidechain | 201 | 10.7 | 18 | 9.0 | 1.0 | 5 | 2.5 | 0.3 |
| Long range (i-j ≥5) | 11 | 0.6 | 5 | 45.5 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 1 | 0.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 4 | 0.2 | 1 | 25.0 | 0.1 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 6 | 0.3 | 4 | 66.7 | 0.2 | 0 | 0.0 | 0.0 |
| 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 | 20 | 1.1 | 9 | 45.0 | 0.5 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 1887 | 100.0 | 82 | 4.3 | 4.3 | 18 | 1.0 | 1.0 |
| Backbone-Backbone | 349 | 18.5 | 15 | 4.3 | 0.8 | 8 | 2.3 | 0.4 |
| Backbone-Sidechain | 887 | 47.0 | 37 | 4.2 | 2.0 | 3 | 0.3 | 0.2 |
| Sidechain-Sidechain | 651 | 34.5 | 30 | 4.6 | 1.6 | 7 | 1.1 | 0.4 |

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ 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 ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 0 | 9 | 19 | 0 | 0 | 28 | 0.44 | 1.12 | 0.27 | 0.38 |
| 2 | 0 | 9 | 19 | 0 | 0 | 28 | 0.43 | 1.13 | 0.28 | 0.36 |
| 3 | 0 | 9 | 16 | 0 | 0 | 25 | 0.43 | 1.15 | 0.28 | 0.32 |
| 4 | 0 | 11 | 17 | 0 | 0 | 28 | 0.45 | 1.13 | 0.27 | 0.41 |
| 5 | 0 | 10 | 17 | 0 | 0 | 27 | 0.42 | 1.18 | 0.27 | 0.36 |
| 6 | 1 | 9 | 20 | 0 | 0 | 30 | 0.41 | 1.13 | 0.28 | 0.37 |
| 7 | 0 | 10 | 20 | 0 | 0 | 30 | 0.38 | 1.15 | 0.25 | 0.3 |
| 8 | 0 | 10 | 18 | 0 | 0 | 28 | 0.41 | 0.96 | 0.22 | 0.3 |
| 9 | 0 | 12 | 19 | 0 | 0 | 31 | 0.42 | 1.12 | 0.28 | 0.35 |
| 10 | 1 | 9 | 18 | 0 | 0 | 28 | 0.43 | 1.12 | 0.27 | 0.38 |

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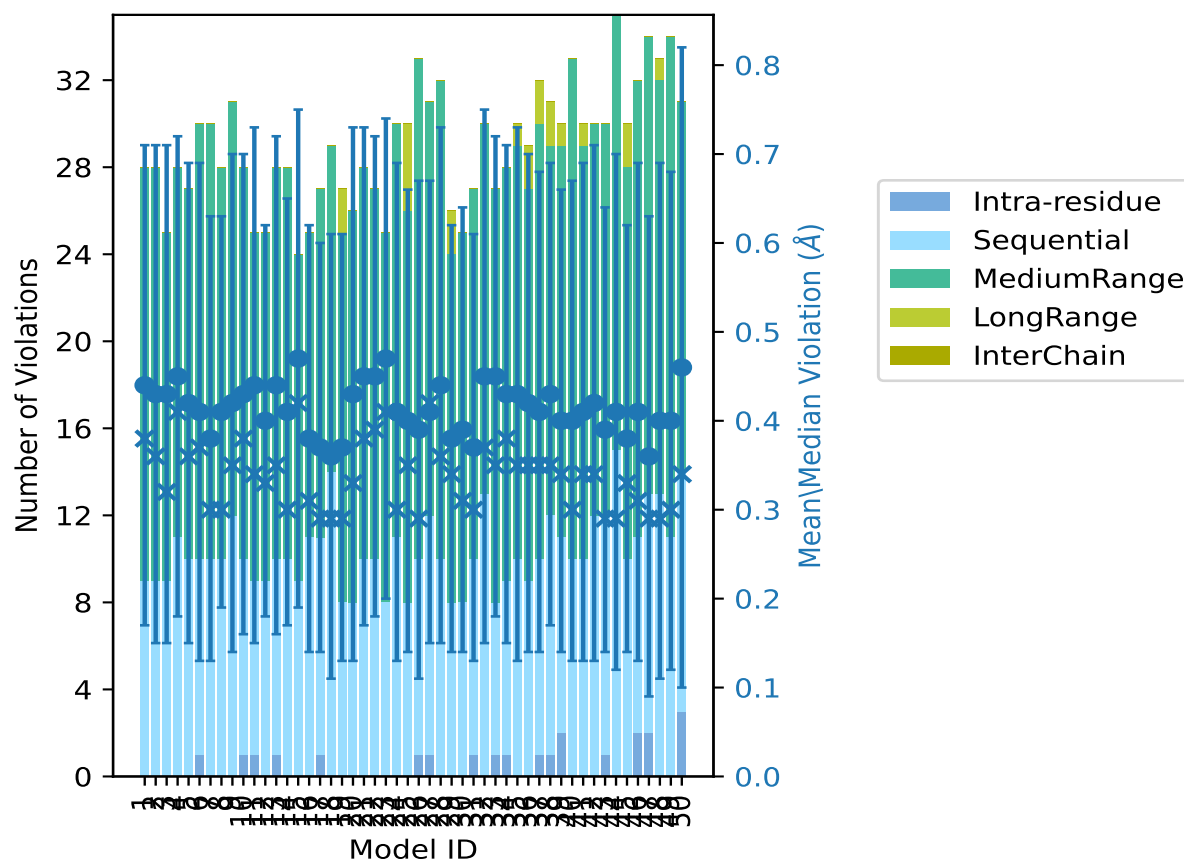
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 1 | 8 | 16 | 0 | 0 | 25 | 0.44 | 1.14 | 0.29 | 0.34 |
| 12 | 0 | 9 | 16 | 0 | 0 | 25 | 0.4 | 0.95 | 0.22 | 0.33 |
| 13 | 1 | 9 | 18 | 0 | 0 | 28 | 0.44 | 1.14 | 0.28 | 0.35 |
| 14 | 0 | 10 | 18 | 0 | 0 | 28 | 0.41 | 1.08 | 0.24 | 0.3 |
| 15 | 0 | 9 | 15 | 0 | 0 | 24 | 0.47 | 1.1 | 0.28 | 0.42 |
| 16 | 0 | 11 | 14 | 0 | 0 | 25 | 0.38 | 1.02 | 0.24 | 0.31 |
| 17 | 1 | 10 | 16 | 0 | 0 | 27 | 0.37 | 0.98 | 0.23 | 0.29 |
| 18 | 0 | 14 | 15 | 0 | 0 | 29 | 0.36 | 1.14 | 0.25 | 0.29 |
| 19 | 0 | 8 | 17 | 2 | 0 | 27 | 0.37 | 1.0 | 0.24 | 0.29 |
| 20 | 0 | 8 | 18 | 0 | 0 | 26 | 0.43 | 1.14 | 0.3 | 0.33 |
| 21 | 0 | 10 | 18 | 0 | 0 | 28 | 0.45 | 1.07 | 0.28 | 0.38 |
| 22 | 0 | 10 | 17 | 0 | 0 | 27 | 0.45 | 1.07 | 0.27 | 0.39 |
| 23 | 0 | 8 | 17 | 0 | 0 | 25 | 0.47 | 1.13 | 0.27 | 0.41 |
| 24 | 0 | 11 | 19 | 0 | 0 | 30 | 0.41 | 1.09 | 0.28 | 0.3 |
| 25 | 0 | 8 | 18 | 4 | 0 | 30 | 0.4 | 1.14 | 0.26 | 0.35 |
| 26 | 1 | 9 | 23 | 0 | 0 | 33 | 0.39 | 1.13 | 0.28 | 0.29 |
| 27 | 1 | 11 | 19 | 0 | 0 | 31 | 0.41 | 1.12 | 0.26 | 0.42 |
| 28 | 0 | 10 | 22 | 0 | 0 | 32 | 0.44 | 1.16 | 0.29 | 0.36 |
| 29 | 0 | 8 | 16 | 2 | 0 | 26 | 0.38 | 1.11 | 0.24 | 0.34 |
| 30 | 0 | 8 | 17 | 0 | 0 | 25 | 0.39 | 1.14 | 0.25 | 0.31 |
| 31 | 1 | 9 | 17 | 0 | 0 | 27 | 0.37 | 1.04 | 0.24 | 0.3 |
| 32 | 0 | 13 | 17 | 0 | 0 | 30 | 0.45 | 1.14 | 0.3 | 0.37 |
| 33 | 1 | 7 | 19 | 0 | 0 | 27 | 0.45 | 1.12 | 0.27 | 0.35 |
| 34 | 1 | 8 | 19 | 0 | 0 | 28 | 0.43 | 1.13 | 0.28 | 0.38 |
| 35 | 0 | 10 | 19 | 1 | 0 | 30 | 0.43 | 1.25 | 0.3 | 0.35 |
| 36 | 0 | 9 | 18 | 2 | 0 | 29 | 0.42 | 1.16 | 0.28 | 0.35 |
| 37 | 1 | 9 | 20 | 2 | 0 | 32 | 0.41 | 1.13 | 0.27 | 0.35 |
| 38 | 1 | 11 | 17 | 2 | 0 | 31 | 0.43 | 1.13 | 0.26 | 0.35 |
| 39 | 2 | 9 | 18 | 1 | 0 | 30 | 0.4 | 1.03 | 0.26 | 0.34 |
| 40 | 0 | 10 | 23 | 0 | 0 | 33 | 0.4 | 1.04 | 0.27 | 0.3 |
| 41 | 0 | 10 | 19 | 1 | 0 | 30 | 0.41 | 1.22 | 0.28 | 0.34 |
| 42 | 0 | 12 | 18 | 0 | 0 | 30 | 0.42 | 1.15 | 0.29 | 0.34 |
| 43 | 1 | 11 | 18 | 0 | 0 | 30 | 0.39 | 1.06 | 0.25 | 0.29 |
| 44 | 0 | 15 | 20 | 0 | 0 | 35 | 0.41 | 1.19 | 0.29 | 0.29 |
| 45 | 0 | 10 | 18 | 2 | 0 | 30 | 0.38 | 1.15 | 0.24 | 0.33 |
| 46 | 2 | 9 | 21 | 0 | 0 | 32 | 0.41 | 1.12 | 0.28 | 0.31 |
| 47 | 2 | 11 | 21 | 0 | 0 | 34 | 0.36 | 1.13 | 0.27 | 0.29 |
| 48 | 0 | 13 | 19 | 1 | 0 | 33 | 0.4 | 1.17 | 0.29 | 0.29 |
| 49 | 0 | 11 | 23 | 0 | 0 | 34 | 0.4 | 1.15 | 0.28 | 0.3 |
| 50 | 3 | 11 | 17 | 0 | 0 | 31 | 0.46 | 1.62 | 0.36 | 0.34 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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, 1794(IR:732, SQ:484, MR:572, LR:6, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-----|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 3 | 3 | 13 | 0 | 0 | 19 | 1 | 2.0 |
| 0 | 3 | 5 | 2 | 0 | 10 | 2 | 4.0 |
| 3 | 0 | 1 | 0 | 0 | 4 | 3 | 6.0 |
| 0 | 0 | 0 | 1 | 0 | 1 | 4 | 8.0 |

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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 0 | 0 | 0 | 0 | 0 | 5 | 10.0 |
| 0 | 0 | 0 | 2 | 0 | 2 | 6 | 12.0 |
| 0 | 0 | 3 | 0 | 0 | 3 | 7 | 14.0 |
| 0 | 0 | 2 | 0 | 0 | 2 | 8 | 16.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 9 | 18.0 |
| 1 | 0 | 0 | 0 | 0 | 1 | 10 | 20.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 11 | 22.0 |
| 0 | 1 | 0 | 0 | 0 | 1 | 12 | 24.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 13 | 26.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 14 | 28.0 |
| 0 | 0 | 2 | 0 | 0 | 2 | 15 | 30.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 16 | 32.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 17 | 34.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 18 | 36.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 19 | 38.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 20 | 40.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 21 | 42.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 22 | 44.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 23 | 46.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 24 | 48.0 |
| 0 | 2 | 0 | 0 | 0 | 2 | 25 | 50.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 26 | 52.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 27 | 54.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 28 | 56.0 |
| 0 | 0 | 2 | 0 | 0 | 2 | 29 | 58.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 30 | 60.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 31 | 62.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 32 | 64.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 33 | 66.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 34 | 68.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 35 | 70.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 36 | 72.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 37 | 74.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 38 | 76.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 39 | 78.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 40 | 80.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 41 | 82.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 42 | 84.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 43 | 86.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 44 | 88.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 45 | 90.0 |

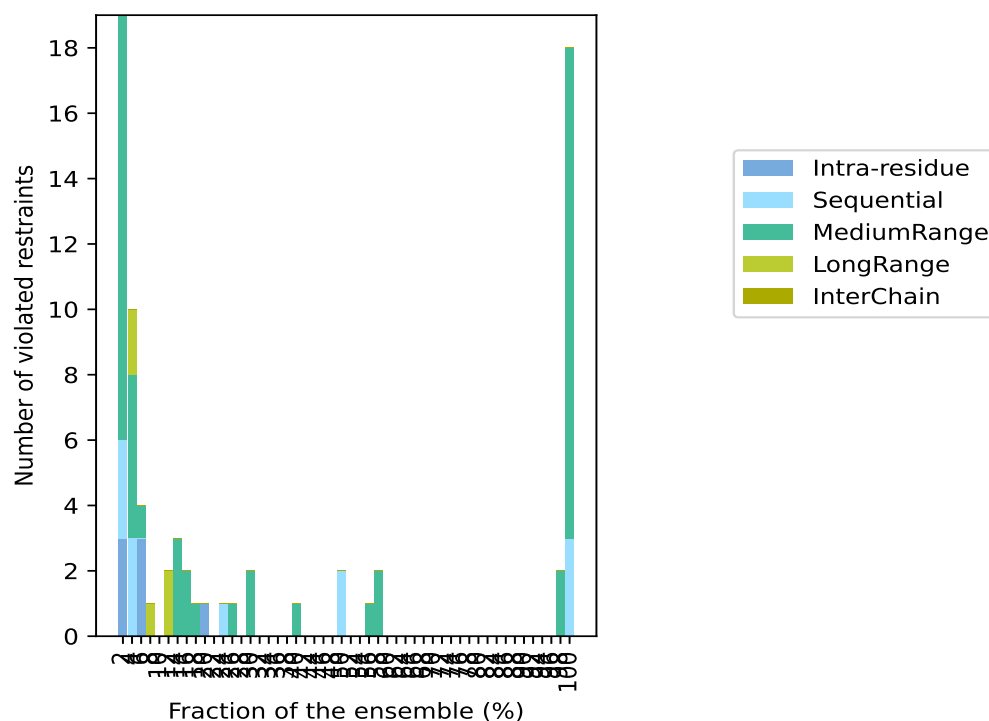
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 0 | 0 | 0 | 0 | 0 | 46 | 92.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 47 | 94.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 48 | 96.0 |
| 0 | 0 | 2 | 0 | 0 | 2 | 49 | 98.0 |
| 0 | 3 | 15 | 0 | 0 | 18 | 50 | 100.0 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

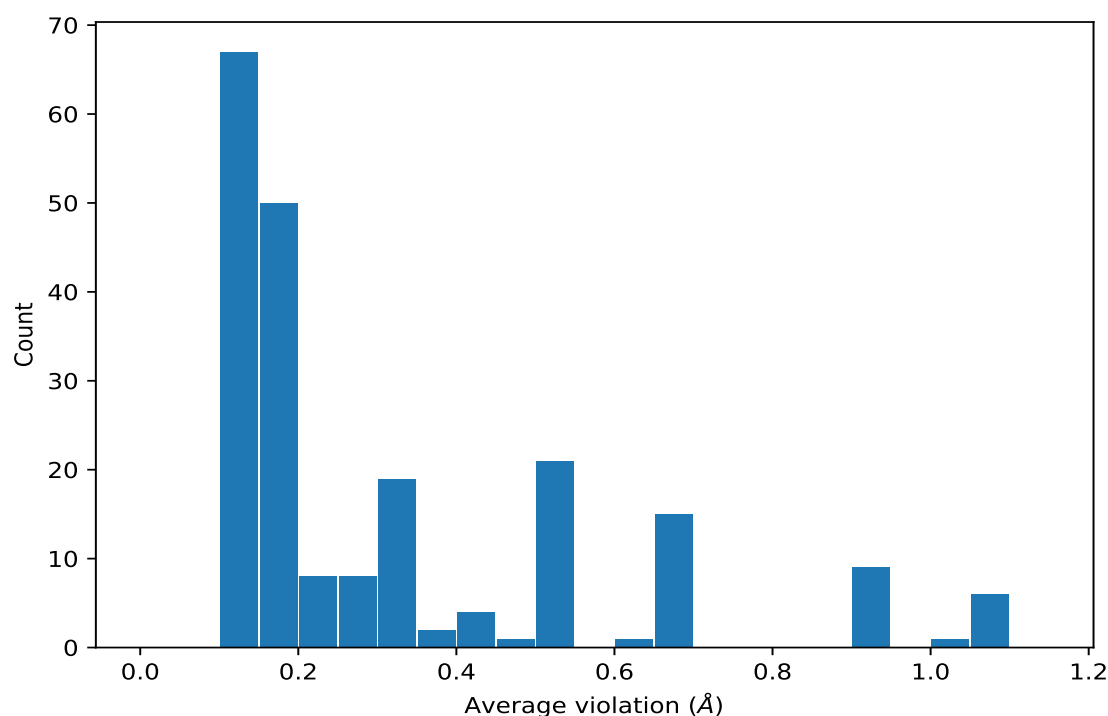
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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



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 ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 50 | 1.08 | 0.06 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 50 | 1.08 | 0.06 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 50 | 1.08 | 0.06 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD12 | 1:16:A:LEU:H | 50 | 1.08 | 0.06 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 50 | 1.08 | 0.06 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 50 | 1.08 | 0.06 | 1.08 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 50 | 0.94 | 0.05 | 0.96 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 50 | 0.69 | 0.02 | 0.69 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 50 | 0.69 | 0.02 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 50 | 0.69 | 0.02 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 50 | 0.69 | 0.02 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 50 | 0.69 | 0.02 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 50 | 0.69 | 0.02 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 50 | 0.68 | 0.03 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 50 | 0.68 | 0.03 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 50 | 0.68 | 0.03 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 50 | 0.68 | 0.03 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 50 | 0.68 | 0.03 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 50 | 0.68 | 0.03 | 0.67 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 50 | 0.66 | 0.05 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 50 | 0.66 | 0.05 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 50 | 0.66 | 0.05 | 0.66 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 50 | 0.54 | 0.15 | 0.51 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 50 | 0.54 | 0.15 | 0.51 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 50 | 0.54 | 0.15 | 0.51 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1827) | 1:8:A:VAL:HG11 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1827) | 1:8:A:VAL:HG12 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1827) | 1:8:A:VAL:HG13 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1827) | 1:8:A:VAL:HG21 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1827) | 1:8:A:VAL:HG22 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1827) | 1:8:A:VAL:HG23 | 1:6:A:TRP:HE3 | 50 | 0.52 | 0.03 | 0.53 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 50 | 0.46 | 0.05 | 0.45 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 50 | 0.39 | 0.03 | 0.39 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 50 | 0.39 | 0.03 | 0.39 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 50 | 0.3 | 0.02 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 50 | 0.3 | 0.02 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 50 | 0.3 | 0.02 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 50 | 0.3 | 0.02 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 50 | 0.3 | 0.02 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 50 | 0.3 | 0.02 | 0.3 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 50 | 0.29 | 0.0 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 50 | 0.29 | 0.0 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 50 | 0.29 | 0.02 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 50 | 0.29 | 0.02 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 50 | 0.29 | 0.02 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 50 | 0.29 | 0.02 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 50 | 0.29 | 0.02 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 50 | 0.29 | 0.02 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 50 | 0.18 | 0.01 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 50 | 0.18 | 0.01 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 50 | 0.18 | 0.01 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 50 | 0.18 | 0.01 | 0.17 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 49 | 0.41 | 0.06 | 0.39 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 49 | 0.41 | 0.06 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 49 | 0.41 | 0.06 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 49 | 0.41 | 0.06 | 0.39 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 44 | 1.01 | 0.27 | 1.12 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 41 | 0.6 | 0.16 | 0.62 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 29 | 0.21 | 0.08 | 0.19 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 29 | 0.21 | 0.08 | 0.19 |
| (1,1745) | 1:25:A:LEU:HD22 | 1:24:A:TRP:HE3 | 29 | 0.17 | 0.03 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD11 | 1:24:A:TRP:HE3 | 29 | 0.17 | 0.03 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 29 | 0.17 | 0.03 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD21 | 1:24:A:TRP:HE3 | 29 | 0.17 | 0.03 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD23 | 1:24:A:TRP:HE3 | 29 | 0.17 | 0.03 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD12 | 1:24:A:TRP:HE3 | 29 | 0.17 | 0.03 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD11 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD11 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD12 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD12 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD13 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD13 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD21 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD21 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD22 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD22 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD23 | 1:28:A:TYR:HE1 | 28 | 0.19 | 0.03 | 0.18 |
| (1,1711) | 1:25:A:LEU:HD23 | 1:28:A:TYR:HE2 | 28 | 0.19 | 0.03 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 25 | 0.52 | 0.13 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 25 | 0.52 | 0.13 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 25 | 0.52 | 0.13 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE1 | 25 | 0.52 | 0.13 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE2 | 25 | 0.52 | 0.13 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 25 | 0.52 | 0.13 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 25 | 0.52 | 0.13 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 25 | 0.52 | 0.13 | 0.51 |
| (1,1867) | 1:23:A:PHE:HE1 | 1:24:A:TRP:H | 25 | 0.52 | 0.13 | 0.51 |
| (1,1867) | 1:23:A:PHE:HE2 | 1:24:A:TRP:H | 25 | 0.52 | 0.13 | 0.51 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 20 | 0.12 | 0.02 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 20 | 0.12 | 0.02 | 0.11 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 18 | 0.34 | 0.1 | 0.34 |
| (1,1789) | 1:17:A:THR:HB | 1:16:A:LEU:H | 15 | 0.16 | 0.03 | 0.16 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 15 | 0.16 | 0.03 | 0.16 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 15 | 0.12 | 0.02 | 0.11 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 15 | 0.12 | 0.02 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 13 | 0.17 | 0.05 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 13 | 0.17 | 0.05 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 13 | 0.17 | 0.05 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 13 | 0.17 | 0.05 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 13 | 0.17 | 0.05 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 13 | 0.17 | 0.05 | 0.16 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 12 | 0.15 | 0.02 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 12 | 0.15 | 0.02 | 0.14 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 10 | 0.11 | 0.03 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 10 | 0.11 | 0.03 | 0.1 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD1 | 9 | 0.24 | 0.12 | 0.22 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD2 | 9 | 0.24 | 0.12 | 0.22 |
| (1,1722) | 1:25:A:LEU:HD13 | 1:21:A:PHE:HD1 | 9 | 0.24 | 0.12 | 0.22 |
| (1,1722) | 1:25:A:LEU:HD13 | 1:21:A:PHE:HD2 | 9 | 0.24 | 0.12 | 0.22 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD1 | 9 | 0.24 | 0.12 | 0.22 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD2 | 9 | 0.24 | 0.12 | 0.22 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 8 | 0.16 | 0.05 | 0.16 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 8 | 0.11 | 0.01 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 8 | 0.11 | 0.01 | 0.11 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:24:A:TRP:HA | 7 | 0.16 | 0.04 | 0.17 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HA | 7 | 0.16 | 0.04 | 0.17 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 7 | 0.13 | 0.02 | 0.13 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 7 | 0.13 | 0.02 | 0.13 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 7 | 0.12 | 0.02 | 0.12 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 6 | 0.3 | 0.11 | 0.34 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD2 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD3 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD2 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD3 | 4 | 0.12 | 0.01 | 0.12 |
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE1 | 3 | 0.13 | 0.02 | 0.12 |
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE2 | 3 | 0.13 | 0.02 | 0.12 |
| (1,405) | 1:23:A:PHE:HE1 | 1:23:A:PHE:H | 3 | 0.13 | 0.02 | 0.12 |
| (1,405) | 1:23:A:PHE:HE2 | 1:23:A:PHE:H | 3 | 0.13 | 0.02 | 0.12 |
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD1 | 3 | 0.12 | 0.02 | 0.12 |
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD2 | 3 | 0.12 | 0.02 | 0.12 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD1 | 3 | 0.12 | 0.02 | 0.12 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD2 | 3 | 0.12 | 0.02 | 0.12 |
| (2,17) | 1:22:A:GLY:O | 1:26:A:PHE:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,98) | 1:6:A:TRP:HD1 | 1:6:A:TRP:HE3 | 3 | 0.1 | 0.0 | 0.1 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ1 | 2 | 0.15 | 0.04 | 0.15 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ2 | 2 | 0.15 | 0.04 | 0.15 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,1623) | 1:23:A:PHE:HA | 1:19:A:LEU:HA | 2 | 0.12 | 0.01 | 0.12 |
| (1,1179) | 1:5:A:ILE:H | 1:3:A:HIS:HE1 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1798) | 1:20:A:ALA:H | 1:22:A:GLY:HA2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1798) | 1:20:A:ALA:H | 1:22:A:GLY:HA3 | 2 | 0.12 | 0.0 | 0.12 |

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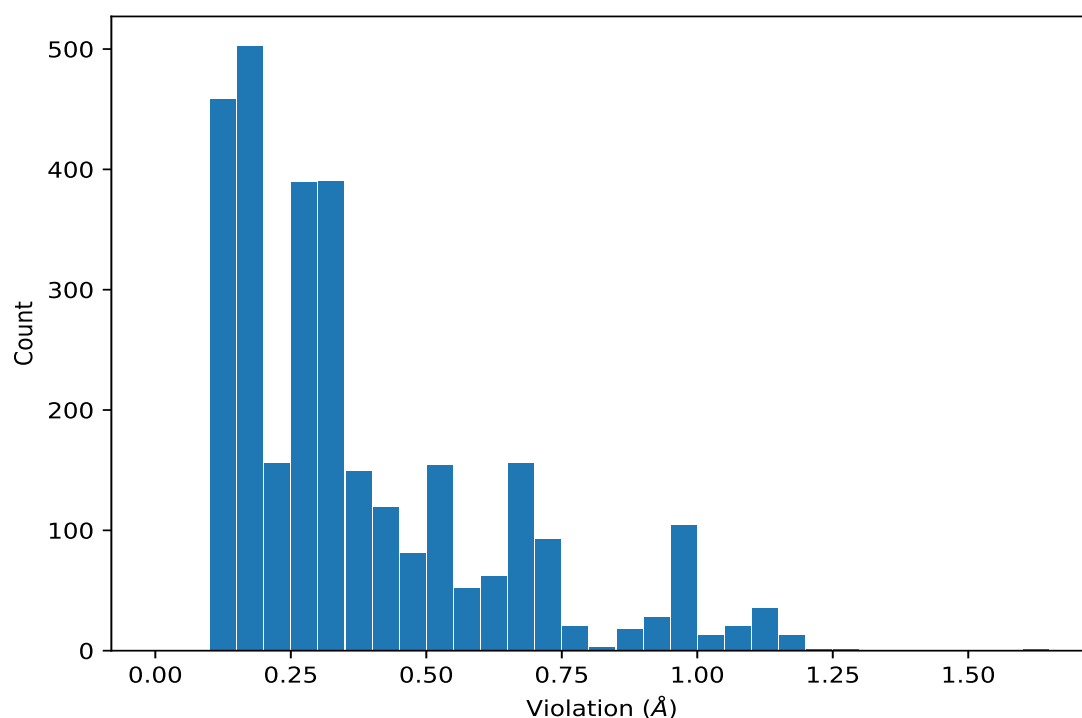
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1079) | 1:27:A:LYS:HG2 | 1:26:A:PHE:HD1 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1079) | 1:27:A:LYS:HG2 | 1:26:A:PHE:HD2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1079) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HD1 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1079) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HD2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1085) | 1:26:A:PHE:HD1 | 1:27:A:LYS:HG2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1085) | 1:26:A:PHE:HD1 | 1:27:A:LYS:HG3 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1085) | 1:26:A:PHE:HD2 | 1:27:A:LYS:HG2 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1085) | 1:26:A:PHE:HD2 | 1:27:A:LYS:HG3 | 2 | 0.11 | 0.01 | 0.11 |
| (1,1286) | 1:7:A:GLU:HB2 | 1:4:A:THR:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,1286) | 1:7:A:GLU:HB3 | 1:4:A:THR:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG11 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG12 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG13 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG11 | 1:3:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG12 | 1:3:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG13 | 1:3:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG21 | 1:3:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG22 | 1:3:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG23 | 1:3:A:HIS:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG11 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG12 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG13 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG23 | 2 | 0.11 | 0.0 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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) |
|----------|-----------------|--------------|----------|---------------|
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 50 | 1.62 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 35 | 1.25 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 41 | 1.22 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 44 | 1.19 |
| (1,1753) | 1:15:A:LEU:HD12 | 1:16:A:LEU:H | 5 | 1.18 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 50 | 1.17 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 48 | 1.17 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 35 | 1.17 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 36 | 1.16 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 28 | 1.16 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 3 | 1.15 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 42 | 1.15 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 7 | 1.15 |
| (1,1753) | 1:15:A:LEU:HD12 | 1:16:A:LEU:H | 45 | 1.15 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 49 | 1.15 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 50 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 11 | 1.14 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 20 | 1.14 |
| (1,1753) | 1:15:A:LEU:HD12 | 1:16:A:LEU:H | 13 | 1.14 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 18 | 1.14 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 20 | 1.14 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 25 | 1.14 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 30 | 1.14 |
| (1,1753) | 1:15:A:LEU:HD12 | 1:16:A:LEU:H | 32 | 1.14 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 4 | 1.13 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 23 | 1.13 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 26 | 1.13 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 37 | 1.13 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 38 | 1.13 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 2 | 1.13 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 6 | 1.13 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 34 | 1.13 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 36 | 1.13 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 37 | 1.13 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 47 | 1.13 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 1 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 2 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 9 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 10 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 13 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 27 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 28 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 46 | 1.12 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 33 | 1.12 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 41 | 1.12 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 46 | 1.12 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 6 | 1.11 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 29 | 1.11 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 15 | 1.1 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 32 | 1.1 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 33 | 1.1 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 24 | 1.09 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 26 | 1.09 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 34 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 1 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 14 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 27 | 1.08 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 44 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 48 | 1.08 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 21 | 1.07 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 9 | 1.07 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 22 | 1.07 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 42 | 1.07 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 22 | 1.06 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 25 | 1.06 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 4 | 1.06 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 15 | 1.06 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 38 | 1.06 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 43 | 1.06 |
| (1,1753) | 1:15:A:LEU:HD11 | 1:16:A:LEU:H | 21 | 1.05 |
| (1,1753) | 1:15:A:LEU:HD13 | 1:16:A:LEU:H | 24 | 1.05 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 40 | 1.04 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 10 | 1.04 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 11 | 1.04 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 31 | 1.04 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 39 | 1.03 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 49 | 1.02 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 3 | 1.02 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 16 | 1.02 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 19 | 1.0 |
| (1,1753) | 1:15:A:LEU:HD22 | 1:16:A:LEU:H | 23 | 1.0 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 20 | 1.0 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 20 | 1.0 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 20 | 1.0 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 6 | 0.99 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 6 | 0.99 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 6 | 0.99 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 17 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 5 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 5 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 5 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 14 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 14 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 14 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 15 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 15 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 15 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 21 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 21 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 21 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 42 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 42 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 42 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 47 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 47 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 47 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 48 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 48 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 48 | 0.98 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 50 | 0.98 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 1 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 1 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 1 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 2 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 2 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 2 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 3 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 3 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 3 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 7 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 7 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 7 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 10 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 10 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 10 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 23 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 23 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 23 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 24 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 24 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 24 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 31 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 31 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 31 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 35 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 35 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 35 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 39 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 39 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 39 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 43 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 43 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 43 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 44 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 44 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 44 | 0.97 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 4 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 4 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 4 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 8 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 8 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 8 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 11 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 11 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 11 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 22 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 22 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 22 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 26 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 26 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 26 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 28 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 28 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 28 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 30 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 30 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 30 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 32 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 32 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 32 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 34 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 34 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 34 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 40 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 40 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 40 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 49 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 49 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 49 | 0.96 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 12 | 0.95 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 12 | 0.95 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 12 | 0.95 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 18 | 0.95 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 18 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 18 | 0.95 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 46 | 0.95 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 46 | 0.95 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 46 | 0.95 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 8 | 0.94 |
| (1,1753) | 1:15:A:LEU:HD21 | 1:16:A:LEU:H | 12 | 0.94 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 9 | 0.94 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 9 | 0.94 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 9 | 0.94 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 39 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 19 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 19 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 19 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 33 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 33 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 33 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 50 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 50 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 50 | 0.93 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 17 | 0.92 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 17 | 0.92 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 17 | 0.92 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 5 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 13 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 13 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 13 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 38 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 38 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 38 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 45 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 45 | 0.9 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 45 | 0.9 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 47 | 0.89 |
| (1,1753) | 1:15:A:LEU:HD23 | 1:16:A:LEU:H | 40 | 0.89 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 36 | 0.89 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 36 | 0.89 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 36 | 0.89 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 37 | 0.89 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 37 | 0.89 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 37 | 0.89 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG21 | 16 | 0.87 |
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG22 | 16 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1730) | 1:9:A:ILE:HD11 | 1:5:A:ILE:HG23 | 16 | 0.87 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 29 | 0.87 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 29 | 0.87 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 29 | 0.87 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 41 | 0.85 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 41 | 0.85 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 41 | 0.85 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 43 | 0.85 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG21 | 27 | 0.81 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG22 | 27 | 0.81 |
| (1,1730) | 1:9:A:ILE:HD13 | 1:5:A:ILE:HG23 | 27 | 0.81 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 35 | 0.78 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 37 | 0.77 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 37 | 0.77 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 32 | 0.77 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 41 | 0.76 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 28 | 0.76 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 28 | 0.76 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 28 | 0.76 |
| (1,1867) | 1:23:A:PHE:HE1 | 1:24:A:TRP:H | 32 | 0.76 |
| (1,1867) | 1:23:A:PHE:HE2 | 1:24:A:TRP:H | 32 | 0.76 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 28 | 0.76 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 28 | 0.76 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 28 | 0.76 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE1 | 32 | 0.76 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE2 | 32 | 0.76 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 38 | 0.76 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 36 | 0.76 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 36 | 0.76 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 28 | 0.76 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 44 | 0.75 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 12 | 0.74 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 12 | 0.74 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 49 | 0.73 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 49 | 0.73 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 49 | 0.73 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 49 | 0.73 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 49 | 0.73 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 49 | 0.73 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 4 | 0.73 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 43 | 0.73 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 44 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 45 | 0.73 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 45 | 0.73 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 46 | 0.73 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 46 | 0.73 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 47 | 0.73 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 42 | 0.72 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 48 | 0.72 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 50 | 0.72 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 50 | 0.72 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 9 | 0.72 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 21 | 0.72 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 24 | 0.72 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 33 | 0.72 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 33 | 0.72 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 38 | 0.72 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 38 | 0.72 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 4 | 0.71 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 4 | 0.71 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 15 | 0.71 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 15 | 0.71 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 44 | 0.71 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 44 | 0.71 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 48 | 0.71 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 48 | 0.71 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 49 | 0.71 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 9 | 0.71 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 9 | 0.71 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 50 | 0.71 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 50 | 0.71 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 14 | 0.71 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 28 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 7 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 7 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 8 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 8 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 9 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 9 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 10 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 10 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 11 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 11 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 13 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 13 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 14 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 14 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 21 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 21 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 22 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 22 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 24 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 24 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 28 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 28 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 30 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 30 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 33 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 33 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 34 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 34 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 40 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 40 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 42 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 42 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 43 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 43 | 0.7 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 42 | 0.7 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 48 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 5 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 5 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 7 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 7 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 8 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 8 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 13 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 13 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 18 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 18 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 24 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 24 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 47 | 0.7 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 47 | 0.7 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 45 | 0.7 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 1 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 1 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 2 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 2 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 3 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 3 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 6 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 6 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 18 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 18 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 20 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 20 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 23 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 23 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 26 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 26 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 31 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 31 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 32 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 32 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 35 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 35 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 39 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 39 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 46 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 46 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 47 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 47 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 49 | 0.69 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 49 | 0.69 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 1 | 0.69 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 11 | 0.69 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 15 | 0.69 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 32 | 0.69 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 34 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 4 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 4 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 11 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 11 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 21 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 21 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 30 | 0.69 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 30 | 0.69 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 8 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 5 | 0.68 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 5 | 0.68 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 12 | 0.68 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 12 | 0.68 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 29 | 0.68 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 29 | 0.68 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG21 | 25 | 0.68 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG22 | 25 | 0.68 |
| (1,1730) | 1:9:A:ILE:HD12 | 1:5:A:ILE:HG23 | 25 | 0.68 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 22 | 0.68 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 22 | 0.68 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 41 | 0.68 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 41 | 0.68 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 44 | 0.68 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 44 | 0.68 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 32 | 0.67 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 23 | 0.67 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 23 | 0.67 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 23 | 0.67 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 23 | 0.67 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 23 | 0.67 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 23 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 16 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 16 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 19 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 19 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 37 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 37 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 38 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 38 | 0.67 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 2 | 0.67 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 6 | 0.67 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 14 | 0.67 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 23 | 0.67 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 25 | 0.67 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 47 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 6 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 6 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 10 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 10 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 20 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 20 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 28 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 28 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 31 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 31 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 32 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 32 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 34 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 34 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 40 | 0.67 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 40 | 0.67 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 7 | 0.67 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 44 | 0.67 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 17 | 0.66 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 17 | 0.66 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 27 | 0.66 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 27 | 0.66 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 36 | 0.66 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 36 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 16 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 18 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 19 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 20 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 29 | 0.66 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 35 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 1 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 1 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 2 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 2 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 3 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 3 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 19 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 19 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 23 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 23 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 26 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 26 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 29 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 29 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 35 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 35 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 43 | 0.66 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 43 | 0.66 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 36 | 0.65 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 40 | 0.65 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 40 | 0.65 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 40 | 0.65 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 40 | 0.65 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 40 | 0.65 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 40 | 0.65 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG12 | 25 | 0.65 |
| (1,1788) | 1:5:A:ILE:HD12 | 1:9:A:ILE:HG13 | 25 | 0.65 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG12 | 45 | 0.65 |
| (1,1788) | 1:5:A:ILE:HD13 | 1:9:A:ILE:HG13 | 45 | 0.65 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 7 | 0.65 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 13 | 0.65 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 22 | 0.65 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 36 | 0.65 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 37 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 14 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 14 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 15 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 15 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 16 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 16 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 17 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 17 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 48 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 48 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 49 | 0.65 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 49 | 0.65 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 3 | 0.64 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 11 | 0.64 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 20 | 0.64 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 44 | 0.64 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 44 | 0.64 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 44 | 0.64 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 44 | 0.64 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 44 | 0.64 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 44 | 0.64 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG12 | 41 | 0.64 |
| (1,1788) | 1:5:A:ILE:HD11 | 1:9:A:ILE:HG13 | 41 | 0.64 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 5 | 0.64 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 10 | 0.64 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 40 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG12 | 39 | 0.64 |
| (1,1727) | 1:10:A:ALA:HB3 | 1:9:A:ILE:HG13 | 39 | 0.64 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 42 | 0.64 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 42 | 0.64 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 48 | 0.64 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 4 | 0.63 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 6 | 0.63 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 9 | 0.63 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 23 | 0.63 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 24 | 0.63 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 37 | 0.63 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 38 | 0.63 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 8 | 0.63 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 26 | 0.63 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 27 | 0.63 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 33 | 0.63 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 1 | 0.62 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 2 | 0.62 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 10 | 0.62 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 13 | 0.62 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 15 | 0.62 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 26 | 0.62 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 27 | 0.62 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 30 | 0.62 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 41 | 0.62 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 46 | 0.62 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG12 | 25 | 0.62 |
| (1,1727) | 1:10:A:ALA:HB2 | 1:9:A:ILE:HG13 | 25 | 0.62 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG12 | 27 | 0.62 |
| (1,1727) | 1:10:A:ALA:HB1 | 1:9:A:ILE:HG13 | 27 | 0.62 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 40 | 0.62 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 25 | 0.61 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 34 | 0.61 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 8 | 0.61 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 14 | 0.61 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 3 | 0.61 |
| (1,1779) | 1:12:A:LEU:HD21 | 1:9:A:ILE:H | 28 | 0.61 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 31 | 0.61 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 39 | 0.61 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 22 | 0.61 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 39 | 0.61 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 46 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 42 | 0.6 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 48 | 0.6 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 12 | 0.6 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 45 | 0.6 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 21 | 0.6 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 35 | 0.6 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 21 | 0.59 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 22 | 0.59 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 33 | 0.59 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 46 | 0.59 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 40 | 0.58 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 26 | 0.58 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 17 | 0.58 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 46 | 0.57 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 22 | 0.57 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 22 | 0.57 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 22 | 0.57 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 27 | 0.57 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 22 | 0.57 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 22 | 0.57 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 22 | 0.57 |
| (1,1779) | 1:12:A:LEU:HD23 | 1:9:A:ILE:H | 50 | 0.57 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 15 | 0.57 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 41 | 0.57 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 21 | 0.56 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 21 | 0.56 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 21 | 0.56 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 49 | 0.56 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 21 | 0.56 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 21 | 0.56 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 21 | 0.56 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 36 | 0.56 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 36 | 0.56 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 47 | 0.55 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 49 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 4 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 4 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG11 | 1:6:A:TRP:HE3 | 8 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG12 | 1:6:A:TRP:HE3 | 8 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG13 | 1:6:A:TRP:HE3 | 8 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG21 | 1:6:A:TRP:HE3 | 8 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG22 | 1:6:A:TRP:HE3 | 8 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1827) | 1:8:A:VAL:HG23 | 1:6:A:TRP:HE3 | 8 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG11 | 1:6:A:TRP:HE3 | 11 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG12 | 1:6:A:TRP:HE3 | 11 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG13 | 1:6:A:TRP:HE3 | 11 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG21 | 1:6:A:TRP:HE3 | 11 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG22 | 1:6:A:TRP:HE3 | 11 | 0.55 |
| (1,1827) | 1:8:A:VAL:HG23 | 1:6:A:TRP:HE3 | 11 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 21 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 21 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 24 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 24 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 37 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 37 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 40 | 0.55 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 40 | 0.55 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 12 | 0.55 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 25 | 0.54 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 25 | 0.54 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 25 | 0.54 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 25 | 0.54 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 25 | 0.54 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 25 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 9 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 9 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG11 | 1:6:A:TRP:HE3 | 18 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG12 | 1:6:A:TRP:HE3 | 18 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG13 | 1:6:A:TRP:HE3 | 18 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG21 | 1:6:A:TRP:HE3 | 18 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG22 | 1:6:A:TRP:HE3 | 18 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG23 | 1:6:A:TRP:HE3 | 18 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 22 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 22 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG11 | 1:6:A:TRP:HE3 | 30 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG12 | 1:6:A:TRP:HE3 | 30 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG13 | 1:6:A:TRP:HE3 | 30 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG21 | 1:6:A:TRP:HE3 | 30 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG22 | 1:6:A:TRP:HE3 | 30 | 0.54 |
| (1,1827) | 1:8:A:VAL:HG23 | 1:6:A:TRP:HE3 | 30 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 33 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 33 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 38 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 38 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 44 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 44 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 46 | 0.54 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 46 | 0.54 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 42 | 0.54 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 10 | 0.53 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 10 | 0.53 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 10 | 0.53 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 26 | 0.53 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 26 | 0.53 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 26 | 0.53 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 9 | 0.53 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 10 | 0.53 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 10 | 0.53 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 10 | 0.53 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 26 | 0.53 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 26 | 0.53 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 26 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 5 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 5 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 7 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 7 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 10 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 10 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 12 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 12 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 15 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 15 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 23 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 23 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 28 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 28 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 31 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 31 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 34 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 34 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 42 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 42 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 43 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 43 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 45 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 45 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 48 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 48 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 49 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 49 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 50 | 0.53 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 50 | 0.53 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 21 | 0.53 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 21 | 0.53 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 16 | 0.53 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 13 | 0.52 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 13 | 0.52 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 13 | 0.52 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 13 | 0.52 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 13 | 0.52 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 13 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 1 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 1 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 2 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 2 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 3 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 3 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 13 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 13 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 14 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 14 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 20 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 20 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 26 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 26 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 32 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 32 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 35 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 35 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 39 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 39 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 47 | 0.52 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 47 | 0.52 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 43 | 0.52 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 43 | 0.52 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 5 | 0.52 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 34 | 0.52 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 1 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 1 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 1 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 2 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 2 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 2 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 33 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 33 | 0.51 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 33 | 0.51 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 24 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 1 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 1 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 1 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 2 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 2 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 2 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 33 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 33 | 0.51 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 33 | 0.51 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 6 | 0.51 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 6 | 0.51 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 19 | 0.51 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 19 | 0.51 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 4 | 0.51 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 15 | 0.51 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 24 | 0.51 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 38 | 0.51 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 4 | 0.51 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 15 | 0.51 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 24 | 0.51 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 38 | 0.51 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 7 | 0.5 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 9 | 0.5 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 9 | 0.5 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 9 | 0.5 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 9 | 0.5 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 9 | 0.5 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 9 | 0.5 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 9 | 0.5 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 40 | 0.5 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 44 | 0.5 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 9 | 0.5 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 40 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 44 | 0.5 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 26 | 0.5 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 39 | 0.49 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 4 | 0.49 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 4 | 0.49 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 4 | 0.49 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 44 | 0.49 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 47 | 0.49 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 4 | 0.49 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 4 | 0.49 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 4 | 0.49 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 17 | 0.49 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 17 | 0.49 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 42 | 0.49 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 48 | 0.49 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 42 | 0.49 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 48 | 0.49 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 1 | 0.49 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 11 | 0.49 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 20 | 0.49 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 5 | 0.48 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 6 | 0.48 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 6 | 0.48 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 6 | 0.48 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 16 | 0.48 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 18 | 0.48 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 46 | 0.48 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 6 | 0.48 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 6 | 0.48 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 6 | 0.48 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 16 | 0.48 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 16 | 0.48 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 29 | 0.48 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 29 | 0.48 |
| (1,1779) | 1:12:A:LEU:HD22 | 1:9:A:ILE:H | 17 | 0.48 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 3 | 0.48 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 9 | 0.48 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 25 | 0.48 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 33 | 0.48 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 36 | 0.48 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 27 | 0.47 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 27 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 27 | 0.47 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 34 | 0.47 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 34 | 0.47 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 34 | 0.47 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 32 | 0.47 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 39 | 0.47 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 41 | 0.47 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 27 | 0.47 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 27 | 0.47 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 27 | 0.47 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 34 | 0.47 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 34 | 0.47 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 34 | 0.47 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 41 | 0.47 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 41 | 0.47 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 28 | 0.47 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 28 | 0.47 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 2 | 0.47 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 4 | 0.47 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 10 | 0.47 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 13 | 0.47 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 37 | 0.47 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 38 | 0.47 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 4 | 0.46 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 17 | 0.46 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 31 | 0.46 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 35 | 0.46 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 38 | 0.46 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 50 | 0.46 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 6 | 0.46 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 45 | 0.45 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 30 | 0.45 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 2 | 0.45 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 3 | 0.45 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 5 | 0.45 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 15 | 0.45 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 19 | 0.45 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 29 | 0.45 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 30 | 0.45 |
| (1,1764) | 1:18:A:PHE:H | 1:19:A:LEU:HA | 27 | 0.45 |
| (1,1755) | 1:19:A:LEU:HA | 1:18:A:PHE:H | 27 | 0.45 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 37 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 37 | 0.44 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 37 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 6 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 7 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 11 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 12 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 13 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 14 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 36 | 0.44 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 37 | 0.44 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 37 | 0.44 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 37 | 0.44 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 37 | 0.44 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 14 | 0.44 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 27 | 0.44 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 39 | 0.44 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 14 | 0.44 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 27 | 0.44 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 39 | 0.44 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 8 | 0.44 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 8 | 0.44 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD1 | 27 | 0.44 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD2 | 27 | 0.44 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 18 | 0.44 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 19 | 0.43 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 29 | 0.43 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 31 | 0.43 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 39 | 0.43 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 10 | 0.43 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 20 | 0.43 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 23 | 0.43 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 28 | 0.43 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 33 | 0.43 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 7 | 0.43 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 7 | 0.43 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 1 | 0.42 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 8 | 0.42 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 34 | 0.42 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 45 | 0.42 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 27 | 0.42 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 27 | 0.42 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 16 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 17 | 0.42 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 28 | 0.42 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 16 | 0.42 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 17 | 0.42 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 28 | 0.42 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 14 | 0.42 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 14 | 0.42 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 43 | 0.41 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 23 | 0.41 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 35 | 0.41 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 40 | 0.41 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 42 | 0.41 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 23 | 0.41 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 35 | 0.41 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 40 | 0.41 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 42 | 0.41 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 12 | 0.41 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 31 | 0.41 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 35 | 0.41 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 41 | 0.41 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 12 | 0.41 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 31 | 0.41 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 35 | 0.41 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 41 | 0.41 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 22 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 36 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 36 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 36 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 36 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 36 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 36 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 37 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 37 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 37 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 37 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 37 | 0.4 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 37 | 0.4 |
| (1,1827) | 1:9:A:ILE:HG12 | 1:6:A:TRP:HE3 | 25 | 0.4 |
| (1,1827) | 1:9:A:ILE:HG13 | 1:6:A:TRP:HE3 | 25 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 36 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 36 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 36 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 36 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 36 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 36 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 37 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 37 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 37 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 37 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 37 | 0.4 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 37 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 1 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 11 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 18 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 19 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 20 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 29 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 32 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 43 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 48 | 0.4 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 49 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 1 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 11 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 18 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 19 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 20 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 29 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 32 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 43 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 48 | 0.4 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 49 | 0.4 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 5 | 0.4 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 50 | 0.4 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 5 | 0.4 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 50 | 0.4 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 49 | 0.4 |
| (2,9) | 1:17:A:THR:O | 1:21:A:PHE:H | 26 | 0.39 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 38 | 0.39 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 38 | 0.39 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 38 | 0.39 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 21 | 0.39 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 38 | 0.39 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 38 | 0.39 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 38 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 2 | 0.39 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 3 | 0.39 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 8 | 0.39 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 15 | 0.39 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 22 | 0.39 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 34 | 0.39 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 44 | 0.39 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 2 | 0.39 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 3 | 0.39 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 8 | 0.39 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 15 | 0.39 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 22 | 0.39 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 34 | 0.39 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 44 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 10 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 17 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 19 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 22 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 30 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 39 | 0.39 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 46 | 0.39 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 10 | 0.39 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 17 | 0.39 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 19 | 0.39 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 22 | 0.39 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 30 | 0.39 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 39 | 0.39 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 46 | 0.39 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 42 | 0.38 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 48 | 0.38 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 25 | 0.38 |
| (1,1861) | 1:18:A:PHE:HE2 | 1:19:A:LEU:H | 40 | 0.38 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 6 | 0.38 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 10 | 0.38 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 21 | 0.38 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 24 | 0.38 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 30 | 0.38 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 31 | 0.38 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 6 | 0.38 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 10 | 0.38 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 21 | 0.38 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 24 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 30 | 0.38 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 31 | 0.38 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 23 | 0.38 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 29 | 0.38 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 34 | 0.38 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 23 | 0.38 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 29 | 0.38 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 34 | 0.38 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 27 | 0.38 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 7 | 0.37 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 25 | 0.37 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 46 | 0.37 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 47 | 0.37 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 7 | 0.37 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 25 | 0.37 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 46 | 0.37 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 47 | 0.37 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 35 | 0.37 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 41 | 0.37 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 6 | 0.37 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 32 | 0.37 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 6 | 0.37 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 32 | 0.37 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD1 | 49 | 0.37 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD2 | 49 | 0.37 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 4 | 0.36 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 5 | 0.36 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 26 | 0.36 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 36 | 0.36 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 41 | 0.36 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 4 | 0.36 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 5 | 0.36 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 26 | 0.36 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 36 | 0.36 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 41 | 0.36 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 1 | 0.36 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 45 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 13 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 13 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 13 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 13 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 13 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 13 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 29 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 29 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 29 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 29 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 29 | 0.36 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 29 | 0.36 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 1 | 0.36 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 45 | 0.36 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD1 | 24 | 0.36 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD2 | 24 | 0.36 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 43 | 0.35 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 38 | 0.35 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 38 | 0.35 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 38 | 0.35 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 38 | 0.35 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 38 | 0.35 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 38 | 0.35 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 38 | 0.35 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 38 | 0.35 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 38 | 0.35 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 38 | 0.35 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 38 | 0.35 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 38 | 0.35 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 9 | 0.35 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 33 | 0.35 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 37 | 0.35 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 38 | 0.35 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 45 | 0.35 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 50 | 0.35 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 9 | 0.35 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 33 | 0.35 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 37 | 0.35 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 38 | 0.35 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 45 | 0.35 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 50 | 0.35 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 50 | 0.35 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 13 | 0.35 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 25 | 0.35 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 36 | 0.35 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 37 | 0.35 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 33 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 33 | 0.35 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 33 | 0.35 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 33 | 0.35 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 33 | 0.35 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 33 | 0.35 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 13 | 0.35 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 25 | 0.35 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 36 | 0.35 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 37 | 0.35 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 37 | 0.35 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 37 | 0.35 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 37 | 0.35 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 37 | 0.35 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 37 | 0.35 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 37 | 0.35 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 12 | 0.34 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 50 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 45 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 45 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 45 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 45 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 45 | 0.34 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 45 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 45 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 45 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 45 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 45 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 45 | 0.34 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 45 | 0.34 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 13 | 0.34 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 13 | 0.34 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 11 | 0.34 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 18 | 0.34 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 33 | 0.34 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 27 | 0.34 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 27 | 0.34 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 27 | 0.34 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 27 | 0.34 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 27 | 0.34 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 27 | 0.34 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 11 | 0.34 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 18 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 33 | 0.34 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 36 | 0.34 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 36 | 0.34 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 36 | 0.34 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 36 | 0.34 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 36 | 0.34 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 36 | 0.34 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 19 | 0.34 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 35 | 0.33 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 41 | 0.33 |
| (1,1803) | 1:12:A:LEU:HA | 1:9:A:ILE:HA | 12 | 0.33 |
| (1,1801) | 1:9:A:ILE:HA | 1:12:A:LEU:HA | 12 | 0.33 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 2 | 0.33 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 16 | 0.33 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 20 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 4 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 4 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 4 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 4 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 4 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 4 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 9 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 9 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 9 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 9 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 9 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 9 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 25 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 25 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 25 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 25 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 25 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 25 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 50 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 50 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 50 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 50 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 50 | 0.33 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 50 | 0.33 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 2 | 0.33 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 16 | 0.33 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 20 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 12 | 0.33 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 12 | 0.33 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 12 | 0.33 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 12 | 0.33 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 12 | 0.33 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 12 | 0.33 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 29 | 0.33 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 3 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 44 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 44 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 44 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 44 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 44 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 44 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 48 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 48 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 48 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 48 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 48 | 0.32 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 48 | 0.32 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 3 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 38 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 38 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 38 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 38 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 38 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 38 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 45 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 45 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 45 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 45 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 45 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 45 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 46 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 46 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 46 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 46 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 46 | 0.32 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 46 | 0.32 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 31 | 0.32 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 47 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 6 | 0.31 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 6 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 6 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 6 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 6 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 6 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 7 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 7 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 7 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 7 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 7 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 7 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 8 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 8 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 8 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 8 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 8 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 8 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 14 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 14 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 14 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 14 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 14 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 14 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 15 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 15 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 15 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 15 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 15 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 15 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 16 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 16 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 16 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 16 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 16 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 16 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 21 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 21 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 21 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 21 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 21 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 21 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 24 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 24 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 24 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 24 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 24 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 24 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 28 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 28 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 28 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 28 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 28 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 28 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 42 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 42 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 42 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 42 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 42 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 42 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 43 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 43 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 43 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 43 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 43 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 43 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 47 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 47 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 47 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 47 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 47 | 0.31 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 47 | 0.31 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 47 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 9 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 9 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 9 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 9 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 9 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 9 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 33 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 33 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 33 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 33 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 33 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 33 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 47 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 47 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 47 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 47 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 47 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 47 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 50 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 50 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 50 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 50 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 50 | 0.31 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 50 | 0.31 |
| (1,1708) | 1:25:A:LEU:HD13 | 1:26:A:PHE:HZ | 30 | 0.31 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 8 | 0.3 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 14 | 0.3 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 20 | 0.3 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 27 | 0.3 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 39 | 0.3 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 41 | 0.3 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 14 | 0.3 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 20 | 0.3 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 27 | 0.3 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 39 | 0.3 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 41 | 0.3 |
| (1,1791) | 1:26:A:PHE:HA | 1:29:A:LEU:H | 46 | 0.3 |
| (1,1764) | 1:18:A:PHE:H | 1:16:A:LEU:HA | 49 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 1 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 1 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 1 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 1 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 1 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 1 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 2 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 2 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 2 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 2 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 2 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 2 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 3 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 3 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 3 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 3 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 3 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 3 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 5 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 5 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 5 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 5 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 5 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 5 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 10 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 10 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 10 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 10 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 10 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 10 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 11 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 11 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 11 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 11 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 11 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 11 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 20 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 20 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 20 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 20 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 20 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 20 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 22 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 22 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 22 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 22 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 22 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 22 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 23 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 23 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 23 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 23 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 23 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 23 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 26 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 26 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 26 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 26 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 26 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 26 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 30 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 30 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 30 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 30 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 30 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 30 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 31 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 31 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 31 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 31 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 31 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 31 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 32 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 32 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 32 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 32 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 32 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 32 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 34 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 34 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 34 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 34 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 34 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 34 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 35 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 35 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 35 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 35 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 35 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 35 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 39 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 39 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 39 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 39 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 39 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 39 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 40 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 40 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 40 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 40 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 40 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 40 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 46 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 46 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 46 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 46 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 46 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 46 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 49 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 49 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 49 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 49 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 49 | 0.3 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 49 | 0.3 |
| (1,1755) | 1:16:A:LEU:HA | 1:18:A:PHE:H | 49 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 4 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 4 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 4 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 4 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 4 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 4 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 5 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 5 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 5 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 5 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 5 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 5 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 7 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 7 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 7 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 7 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 7 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 7 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 8 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 8 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 8 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 8 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 8 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 8 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 11 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 11 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 11 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 11 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 11 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 11 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 13 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 13 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 13 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 13 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 13 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 13 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 18 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 18 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 18 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 18 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 18 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 18 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 21 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 21 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 21 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 21 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 21 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 21 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 24 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 24 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 24 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 24 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 24 | 0.3 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 24 | 0.3 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 8 | 0.29 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 14 | 0.29 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 46 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 1 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 2 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 3 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 4 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 5 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 6 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 7 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 8 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 10 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 11 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 12 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 13 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 15 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 16 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 17 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 18 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 19 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 21 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 22 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 23 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 24 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 25 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 26 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 28 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 29 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 30 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 31 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 32 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 33 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 34 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 35 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 36 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 37 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 40 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 43 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 44 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 45 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 46 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 47 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 48 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 49 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 50 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 1 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 2 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 3 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 4 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 5 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 6 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 7 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 8 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 10 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 11 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 12 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 13 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 15 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 16 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 17 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 18 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 19 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 21 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 22 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 23 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 24 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 25 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 26 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 28 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 29 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 30 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 31 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 32 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 33 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 34 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 35 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 36 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 37 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 40 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 43 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 44 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 45 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 46 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 47 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 48 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 49 | 0.29 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 50 | 0.29 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 8 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 12 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 12 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 12 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 12 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 12 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 12 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 18 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 18 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 18 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 18 | 0.29 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 18 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 18 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 30 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 30 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 30 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 30 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 30 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 30 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 44 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 44 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 44 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 44 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 44 | 0.29 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 44 | 0.29 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 50 | 0.29 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 50 | 0.29 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 50 | 0.29 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 50 | 0.29 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 50 | 0.29 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 50 | 0.29 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 9 | 0.28 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 38 | 0.28 |
| (1,1833) | 1:11:A:GLY:H | 1:12:A:LEU:HA | 42 | 0.28 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 9 | 0.28 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 38 | 0.28 |
| (1,1825) | 1:12:A:LEU:HA | 1:11:A:GLY:H | 42 | 0.28 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 7 | 0.28 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 12 | 0.28 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 17 | 0.28 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 48 | 0.28 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 19 | 0.28 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 19 | 0.28 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 19 | 0.28 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 19 | 0.28 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 19 | 0.28 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 19 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 6 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 6 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 6 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 6 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 6 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 6 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 10 | 0.28 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 10 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 10 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 10 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 10 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 10 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 20 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 20 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 20 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 20 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 20 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 20 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 22 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 22 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 22 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 22 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 22 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 22 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 28 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 28 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 28 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 28 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 28 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 28 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 31 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 31 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 31 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 31 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 31 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 31 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 32 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 32 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 32 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 32 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 32 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 32 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 34 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 34 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 34 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 34 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 34 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 34 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 40 | 0.28 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 40 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 40 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 40 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 40 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 40 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 41 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 41 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 41 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 41 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 41 | 0.28 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 41 | 0.28 |
| (1,1708) | 1:25:A:LEU:HD11 | 1:26:A:PHE:HZ | 24 | 0.28 |
| (1,1867) | 1:27:A:LYS:HZ1 | 1:24:A:TRP:H | 43 | 0.27 |
| (1,1867) | 1:27:A:LYS:HZ2 | 1:24:A:TRP:H | 43 | 0.27 |
| (1,1867) | 1:27:A:LYS:HZ3 | 1:24:A:TRP:H | 43 | 0.27 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ1 | 43 | 0.27 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ2 | 43 | 0.27 |
| (1,1858) | 1:24:A:TRP:H | 1:27:A:LYS:HZ3 | 43 | 0.27 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 14 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 17 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 17 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 17 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 17 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 17 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 17 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 38 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 38 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 38 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 38 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 38 | 0.27 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 38 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 1 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 1 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 1 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 1 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 1 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 1 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 2 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 2 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 2 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 2 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 2 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 2 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 3 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 3 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 3 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 3 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 3 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 3 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 14 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 14 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 14 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 14 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 14 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 14 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 16 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 16 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 16 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 16 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 16 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 16 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 17 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 17 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 17 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 17 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 17 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 17 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 19 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 19 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 19 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 19 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 19 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 19 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 23 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 23 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 23 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 23 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 23 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 23 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 26 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 26 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 26 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 26 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 26 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 26 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 29 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 29 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 29 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 29 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 29 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 29 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 35 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 35 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 35 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 35 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 35 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 35 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 43 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 43 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 43 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 43 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 43 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 43 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 49 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 49 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 49 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 49 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 49 | 0.27 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 49 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 8 | 0.27 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 8 | 0.27 |
| (2,19) | 1:23:A:PHE:O | 1:27:A:LYS:H | 17 | 0.26 |
| (1,1867) | 1:23:A:PHE:HE1 | 1:24:A:TRP:H | 18 | 0.26 |
| (1,1867) | 1:23:A:PHE:HE2 | 1:24:A:TRP:H | 18 | 0.26 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE1 | 18 | 0.26 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE2 | 18 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 5 | 0.26 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 42 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 36 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 36 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 36 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 36 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 36 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 36 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 37 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 37 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 37 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 37 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 37 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 37 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 41 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 41 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 41 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 41 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 41 | 0.26 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 41 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 15 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 15 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 15 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 15 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 15 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 15 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 39 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 39 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 39 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 39 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 39 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 39 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 42 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 42 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 42 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 42 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 42 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 42 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 48 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 48 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 48 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 48 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 48 | 0.26 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 48 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 45 | 0.26 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 45 | 0.26 |
| (1,1080) | 1:27:A:LYS:H | 1:26:A:PHE:HD1 | 46 | 0.26 |
| (1,1080) | 1:27:A:LYS:H | 1:26:A:PHE:HD2 | 46 | 0.26 |
| (1,1867) | 1:23:A:PHE:HE1 | 1:24:A:TRP:H | 16 | 0.25 |
| (1,1867) | 1:23:A:PHE:HE2 | 1:24:A:TRP:H | 16 | 0.25 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE1 | 16 | 0.25 |
| (1,1858) | 1:24:A:TRP:H | 1:23:A:PHE:HE2 | 16 | 0.25 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD11 | 45 | 0.25 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD12 | 45 | 0.25 |
| (1,1762) | 1:9:A:ILE:HG12 | 1:5:A:ILE:HD13 | 45 | 0.25 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD11 | 45 | 0.25 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD12 | 45 | 0.25 |
| (1,1762) | 1:9:A:ILE:HG13 | 1:5:A:ILE:HD13 | 45 | 0.25 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 27 | 0.25 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 27 | 0.25 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 27 | 0.25 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 27 | 0.25 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 27 | 0.25 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 27 | 0.25 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 43 | 0.25 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 43 | 0.25 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 43 | 0.25 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 43 | 0.25 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 43 | 0.25 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 43 | 0.25 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 5 | 0.24 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 39 | 0.24 |
| (1,1745) | 1:25:A:LEU:HD11 | 1:24:A:TRP:HE3 | 43 | 0.24 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB1 | 25 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB2 | 25 | 0.24 |
| (1,1739) | 1:9:A:ILE:HG12 | 1:10:A:ALA:HB3 | 25 | 0.24 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB1 | 25 | 0.24 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB2 | 25 | 0.24 |
| (1,1739) | 1:9:A:ILE:HG13 | 1:10:A:ALA:HB3 | 25 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 7 | 0.24 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 7 | 0.24 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 7 | 0.23 |
| (1,1823) | 1:20:A:ALA:H | 1:21:A:PHE:HD1 | 49 | 0.23 |
| (1,1823) | 1:20:A:ALA:H | 1:21:A:PHE:HD2 | 49 | 0.23 |
| (1,1745) | 1:25:A:LEU:HD22 | 1:24:A:TRP:HE3 | 12 | 0.23 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD1 | 32 | 0.23 |
| (1,1722) | 1:25:A:LEU:HD12 | 1:21:A:PHE:HD2 | 32 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 5 | 0.23 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 5 | 0.23 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 14 | 0.22 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:24:A:TRP:HA | 47 | 0.22 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 24 | 0.22 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 31 | 0.22 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD1 | 44 | 0.22 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD2 | 44 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD11 | 1:28:A:TYR:HE1 | 43 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1711) | 1:25:A:LEU:HD11 | 1:28:A:TYR:HE2 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD12 | 1:28:A:TYR:HE1 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD12 | 1:28:A:TYR:HE2 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD13 | 1:28:A:TYR:HE1 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD13 | 1:28:A:TYR:HE2 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD21 | 1:28:A:TYR:HE1 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD21 | 1:28:A:TYR:HE2 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD22 | 1:28:A:TYR:HE1 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD22 | 1:28:A:TYR:HE2 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD23 | 1:28:A:TYR:HE1 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD23 | 1:28:A:TYR:HE2 | 43 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD11 | 1:28:A:TYR:HE1 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD11 | 1:28:A:TYR:HE2 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD12 | 1:28:A:TYR:HE1 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD12 | 1:28:A:TYR:HE2 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD13 | 1:28:A:TYR:HE1 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD13 | 1:28:A:TYR:HE2 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD21 | 1:28:A:TYR:HE1 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD21 | 1:28:A:TYR:HE2 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD22 | 1:28:A:TYR:HE1 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD22 | 1:28:A:TYR:HE2 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD23 | 1:28:A:TYR:HE1 | 47 | 0.22 |
| (1,1711) | 1:25:A:LEU:HD23 | 1:28:A:TYR:HE2 | 47 | 0.22 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 12 | 0.21 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 36 | 0.21 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 37 | 0.21 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 38 | 0.21 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 36 | 0.21 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 37 | 0.21 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 38 | 0.21 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 36 | 0.21 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 37 | 0.21 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 38 | 0.21 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 36 | 0.21 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 37 | 0.21 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 38 | 0.21 |
| (1,1745) | 1:25:A:LEU:HD23 | 1:24:A:TRP:HE3 | 8 | 0.21 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 14 | 0.21 |
| (1,1745) | 1:25:A:LEU:HD21 | 1:24:A:TRP:HE3 | 28 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 24 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 24 | 0.21 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 24 | 0.21 |
| (1,1708) | 1:25:A:LEU:HD12 | 1:26:A:PHE:HZ | 23 | 0.21 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 7 | 0.2 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 17 | 0.2 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:24:A:TRP:HA | 14 | 0.2 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 45 | 0.2 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 9 | 0.2 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 45 | 0.2 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 45 | 0.2 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 45 | 0.2 |
| (1,1745) | 1:25:A:LEU:HD22 | 1:24:A:TRP:HE3 | 1 | 0.2 |
| (1,1745) | 1:25:A:LEU:HD12 | 1:24:A:TRP:HE3 | 35 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 28 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 28 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 28 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 28 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 28 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 28 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 32 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 32 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 32 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 32 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 32 | 0.2 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 32 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 25 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 25 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 35 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 41 | 0.2 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 41 | 0.2 |
| (2,13) | 1:19:A:LEU:O | 1:23:A:PHE:H | 28 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 4 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 7 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 8 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 9 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 12 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 13 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 24 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 25 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 33 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 41 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 46 | 0.19 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 50 | 0.19 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 19 | 0.19 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 30 | 0.19 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 4 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 43 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 4 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 7 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 8 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 9 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 12 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 13 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 24 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 25 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 33 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 41 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 46 | 0.19 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 50 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 4 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 7 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 8 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 9 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 12 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 13 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 24 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 25 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 33 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 41 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 46 | 0.19 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 50 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 4 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 7 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 8 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 9 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 12 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 13 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 24 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 25 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 33 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 41 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 46 | 0.19 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 50 | 0.19 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 17 | 0.19 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD1 | 28 | 0.19 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD2 | 28 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 23 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 23 | 0.19 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 23 | 0.19 |
| (1,1530) | 1:29:A:LEU:H | 1:32:A:LYS:HB2 | 34 | 0.19 |
| (1,1530) | 1:29:A:LEU:H | 1:32:A:LYS:HB3 | 34 | 0.19 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 28 | 0.19 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 28 | 0.19 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 50 | 0.19 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 50 | 0.19 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ1 | 49 | 0.19 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ2 | 49 | 0.19 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ3 | 49 | 0.19 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 33 | 0.19 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 33 | 0.19 |
| (2,20) | 1:23:A:PHE:O | 1:27:A:LYS:N | 45 | 0.18 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 5 | 0.18 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 11 | 0.18 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 19 | 0.18 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 21 | 0.18 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 30 | 0.18 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 44 | 0.18 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 29 | 0.18 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 45 | 0.18 |
| (1,1789) | 1:17:A:THR:HB | 1:16:A:LEU:H | 44 | 0.18 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 5 | 0.18 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 11 | 0.18 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 19 | 0.18 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 21 | 0.18 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 30 | 0.18 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 44 | 0.18 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 5 | 0.18 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 11 | 0.18 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 19 | 0.18 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 21 | 0.18 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 30 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 44 | 0.18 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 5 | 0.18 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 11 | 0.18 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 19 | 0.18 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 21 | 0.18 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 30 | 0.18 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 44 | 0.18 |
| (1,1745) | 1:25:A:LEU:HD21 | 1:24:A:TRP:HE3 | 18 | 0.18 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 41 | 0.18 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 14 | 0.18 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 14 | 0.18 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 14 | 0.18 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 14 | 0.18 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 14 | 0.18 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 14 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 39 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 48 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 48 | 0.18 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 48 | 0.18 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 30 | 0.17 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 42 | 0.17 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 42 | 0.17 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 48 | 0.17 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 48 | 0.17 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 25 | 0.17 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 25 | 0.17 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 25 | 0.17 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 25 | 0.17 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 25 | 0.17 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 25 | 0.17 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 25 | 0.17 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 25 | 0.17 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 25 | 0.17 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 25 | 0.17 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 25 | 0.17 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 25 | 0.17 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:24:A:TRP:HA | 7 | 0.17 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:24:A:TRP:HA | 8 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 1 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 2 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 3 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 6 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 10 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 14 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 15 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 16 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 17 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 18 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 20 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 22 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 23 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 26 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|--------------|----------|---------------|
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 27 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 28 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 29 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 31 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 32 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 34 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 35 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 39 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 40 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 42 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 43 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 47 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 48 | 0.17 |
| (1,1800) | 1:5:A:ILE:HA | 1:8:A:VAL:HA | 49 | 0.17 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 28 | 0.17 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 24 | 0.17 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 38 | 0.17 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 40 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 1 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 2 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 3 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 6 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 10 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 14 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 15 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 16 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 17 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 18 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 20 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 22 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 23 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 26 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 27 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 28 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 29 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 31 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 32 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 34 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 35 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 39 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 40 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 42 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|--------------|----------|---------------|
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 43 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 47 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 48 | 0.17 |
| (1,1776) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 49 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 1 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 2 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 3 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 6 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 10 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 14 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 15 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 16 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 17 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 18 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 20 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 22 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 23 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 26 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 27 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 28 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 29 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 31 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 32 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 34 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 35 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 39 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 40 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 42 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 43 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 47 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 48 | 0.17 |
| (1,1775) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 49 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 1 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 2 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 3 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 6 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 10 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 14 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 15 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 16 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 17 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 18 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 20 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 22 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 23 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 26 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 27 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 28 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 29 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 31 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 32 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 34 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 35 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 39 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 40 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 42 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 43 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 47 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 48 | 0.17 |
| (1,1774) | 1:8:A:VAL:HA | 1:5:A:ILE:HA | 49 | 0.17 |
| (1,1745) | 1:25:A:LEU:HD12 | 1:24:A:TRP:HE3 | 37 | 0.17 |
| (1,1745) | 1:25:A:LEU:HD23 | 1:24:A:TRP:HE3 | 45 | 0.17 |
| (1,1745) | 1:25:A:LEU:HD11 | 1:24:A:TRP:HE3 | 47 | 0.17 |
| (1,1745) | 1:25:A:LEU:HD21 | 1:24:A:TRP:HE3 | 50 | 0.17 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 44 | 0.17 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 44 | 0.17 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 44 | 0.17 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 44 | 0.17 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 44 | 0.17 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 44 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 1 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 4 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 4 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 6 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 22 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 42 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 42 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 49 | 0.17 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 49 | 0.17 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 44 | 0.17 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 44 | 0.17 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 32 | 0.17 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 32 | 0.17 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 29 | 0.16 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 31 | 0.16 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 39 | 0.16 |
| (2,10) | 1:17:A:THR:O | 1:21:A:PHE:N | 26 | 0.16 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 26 | 0.16 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 26 | 0.16 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 18 | 0.16 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 47 | 0.16 |
| (1,1789) | 1:17:A:THR:HB | 1:16:A:LEU:H | 48 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD11 | 1:24:A:TRP:HE3 | 2 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 6 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD22 | 1:24:A:TRP:HE3 | 7 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD22 | 1:24:A:TRP:HE3 | 32 | 0.16 |
| (1,1745) | 1:25:A:LEU:HD21 | 1:24:A:TRP:HE3 | 44 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 47 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 47 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 47 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 47 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 47 | 0.16 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 47 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 2 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 3 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 9 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 21 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 21 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 36 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 37 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 38 | 0.16 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 38 | 0.16 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 31 | 0.16 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 31 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 19 | 0.15 |
| (2,7) | 1:14:A:ALA:O | 1:18:A:PHE:H | 26 | 0.15 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 27 | 0.15 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 27 | 0.15 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 49 | 0.15 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 15 | 0.15 |
| (1,1789) | 1:17:A:THR:HB | 1:16:A:LEU:H | 42 | 0.15 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 9 | 0.15 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 10 | 0.15 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 38 | 0.15 |
| (1,1529) | 1:29:A:LEU:HA | 1:32:A:LYS:HG2 | 24 | 0.15 |
| (1,1529) | 1:29:A:LEU:HA | 1:32:A:LYS:HG3 | 24 | 0.15 |
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD1 | 43 | 0.15 |
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD2 | 43 | 0.15 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD1 | 43 | 0.15 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD2 | 43 | 0.15 |
| (1,1282) | 1:30:A:GLN:HB2 | 1:32:A:LYS:HE2 | 33 | 0.15 |
| (1,1282) | 1:30:A:GLN:HB2 | 1:32:A:LYS:HE3 | 33 | 0.15 |
| (1,1282) | 1:30:A:GLN:HB3 | 1:32:A:LYS:HE2 | 33 | 0.15 |
| (1,1282) | 1:30:A:GLN:HB3 | 1:32:A:LYS:HE3 | 33 | 0.15 |
| (1,405) | 1:23:A:PHE:HE1 | 1:23:A:PHE:H | 50 | 0.15 |
| (1,405) | 1:23:A:PHE:HE2 | 1:23:A:PHE:H | 50 | 0.15 |
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE1 | 50 | 0.15 |
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE2 | 50 | 0.15 |
| (1,1850) | 1:27:A:LYS:HG3 | 1:30:A:GLN:HB2 | 18 | 0.14 |
| (1,1850) | 1:27:A:LYS:HG3 | 1:30:A:GLN:HB3 | 18 | 0.14 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 49 | 0.14 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 49 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 11 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 11 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 13 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 13 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 20 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 20 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 33 | 0.14 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 33 | 0.14 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 1 | 0.14 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 16 | 0.14 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 26 | 0.14 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 40 | 0.14 |
| (1,1745) | 1:25:A:LEU:HD11 | 1:24:A:TRP:HE3 | 4 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 8 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 8 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 8 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 8 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 8 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 45 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 45 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 45 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 45 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 45 | 0.14 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 45 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE1 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD11 | 1:28:A:TYR:HE2 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE1 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD12 | 1:28:A:TYR:HE2 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE1 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD13 | 1:28:A:TYR:HE2 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE1 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD21 | 1:28:A:TYR:HE2 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE1 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD22 | 1:28:A:TYR:HE2 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE1 | 18 | 0.14 |
| (1,1711) | 1:29:A:LEU:HD23 | 1:28:A:TYR:HE2 | 18 | 0.14 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 26 | 0.14 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 26 | 0.14 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 31 | 0.14 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 31 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 10 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 10 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 11 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 11 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 13 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 13 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 20 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 20 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 44 | 0.14 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 44 | 0.14 |
| (2,17) | 1:22:A:GLY:O | 1:26:A:PHE:H | 35 | 0.13 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 46 | 0.13 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 46 | 0.13 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 10 | 0.13 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 26 | 0.13 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 26 | 0.13 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 27 | 0.13 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 27 | 0.13 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 27 | 0.13 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 43 | 0.13 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:20:A:ALA:H | 46 | 0.13 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 21 | 0.13 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 28 | 0.13 |
| (1,1745) | 1:25:A:LEU:HD13 | 1:24:A:TRP:HE3 | 3 | 0.13 |
| (1,1745) | 1:25:A:LEU:HD21 | 1:24:A:TRP:HE3 | 5 | 0.13 |
| (1,1745) | 1:25:A:LEU:HD12 | 1:24:A:TRP:HE3 | 13 | 0.13 |
| (1,1745) | 1:25:A:LEU:HD12 | 1:24:A:TRP:HE3 | 36 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD2 | 35 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD3 | 35 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD2 | 35 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD3 | 35 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD2 | 48 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD3 | 48 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD2 | 48 | 0.13 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD3 | 48 | 0.13 |
| (1,1623) | 1:23:A:PHE:HA | 1:19:A:LEU:HA | 28 | 0.13 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 48 | 0.13 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 48 | 0.13 |
| (1,1179) | 1:5:A:ILE:H | 1:3:A:HIS:HE1 | 27 | 0.13 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 26 | 0.13 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 26 | 0.13 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 27 | 0.13 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 27 | 0.13 |
| (1,395) | 1:23:A:PHE:H | 1:23:A:PHE:HD1 | 50 | 0.13 |
| (1,395) | 1:23:A:PHE:H | 1:23:A:PHE:HD2 | 50 | 0.13 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 42 | 0.12 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 39 | 0.12 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 39 | 0.12 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 41 | 0.12 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 41 | 0.12 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 50 | 0.12 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 50 | 0.12 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 19 | 0.12 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 19 | 0.12 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 19 | 0.12 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 19 | 0.12 |
| (1,1830) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 19 | 0.12 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG11 | 19 | 0.12 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG12 | 19 | 0.12 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG13 | 19 | 0.12 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG21 | 19 | 0.12 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG22 | 19 | 0.12 |
| (1,1818) | 1:3:A:HIS:HB3 | 1:8:A:VAL:HG23 | 19 | 0.12 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HA | 12 | 0.12 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:24:A:TRP:HA | 45 | 0.12 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 42 | 0.12 |
| (1,1798) | 1:20:A:ALA:H | 1:22:A:GLY:HA2 | 41 | 0.12 |
| (1,1798) | 1:20:A:ALA:H | 1:22:A:GLY:HA3 | 41 | 0.12 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 9 | 0.12 |
| (1,1789) | 1:17:A:THR:HB | 1:14:A:ALA:H | 46 | 0.12 |
| (1,1745) | 1:25:A:LEU:HD12 | 1:24:A:TRP:HE3 | 24 | 0.12 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD1 | 6 | 0.12 |
| (1,1722) | 1:25:A:LEU:HD11 | 1:21:A:PHE:HD2 | 6 | 0.12 |
| (1,1722) | 1:25:A:LEU:HD13 | 1:21:A:PHE:HD1 | 26 | 0.12 |
| (1,1722) | 1:25:A:LEU:HD13 | 1:21:A:PHE:HD2 | 26 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 7 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 7 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 7 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 7 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 7 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 7 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 40 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 40 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 40 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 40 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 40 | 0.12 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 40 | 0.12 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD2 | 41 | 0.12 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD3 | 41 | 0.12 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD2 | 41 | 0.12 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD3 | 41 | 0.12 |
| (1,1623) | 1:23:A:PHE:HA | 1:19:A:LEU:HA | 40 | 0.12 |
| (1,1622) | 1:21:A:PHE:HA | 1:17:A:THR:HA | 49 | 0.12 |
| (1,1605) | 1:18:A:PHE:HA | 1:14:A:ALA:HB1 | 26 | 0.12 |
| (1,1605) | 1:18:A:PHE:HA | 1:14:A:ALA:HB2 | 26 | 0.12 |
| (1,1605) | 1:18:A:PHE:HA | 1:14:A:ALA:HB3 | 26 | 0.12 |
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD1 | 47 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD2 | 47 | 0.12 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD1 | 47 | 0.12 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD2 | 47 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 6 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 6 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 6 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 6 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 6 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 6 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 20 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 20 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 20 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 20 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 20 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 20 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 47 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 47 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 47 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 47 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 47 | 0.12 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 47 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 6 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 6 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 6 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 6 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 6 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 6 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 20 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 20 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 20 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 20 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 20 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 20 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 47 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 47 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 47 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 47 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 47 | 0.12 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 47 | 0.12 |
| (1,1286) | 1:7:A:GLU:HB2 | 1:4:A:THR:H | 37 | 0.12 |
| (1,1286) | 1:7:A:GLU:HB3 | 1:4:A:THR:H | 37 | 0.12 |
| (1,1264) | 1:28:A:TYR:HD1 | 1:30:A:GLN:H | 40 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1264) | 1:28:A:TYR:HD2 | 1:30:A:GLN:H | 40 | 0.12 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD1 | 34 | 0.12 |
| (1,1135) | 1:29:A:LEU:HG | 1:28:A:TYR:HD2 | 34 | 0.12 |
| (1,1085) | 1:26:A:PHE:HD1 | 1:27:A:LYS:HG2 | 18 | 0.12 |
| (1,1085) | 1:26:A:PHE:HD1 | 1:27:A:LYS:HG3 | 18 | 0.12 |
| (1,1085) | 1:26:A:PHE:HD2 | 1:27:A:LYS:HG2 | 18 | 0.12 |
| (1,1085) | 1:26:A:PHE:HD2 | 1:27:A:LYS:HG3 | 18 | 0.12 |
| (1,1079) | 1:27:A:LYS:HG2 | 1:26:A:PHE:HD1 | 18 | 0.12 |
| (1,1079) | 1:27:A:LYS:HG2 | 1:26:A:PHE:HD2 | 18 | 0.12 |
| (1,1079) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HD1 | 18 | 0.12 |
| (1,1079) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HD2 | 18 | 0.12 |
| (1,959) | 1:18:A:PHE:HE1 | 1:19:A:LEU:HD11 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE1 | 1:19:A:LEU:HD12 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE1 | 1:19:A:LEU:HD13 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE1 | 1:19:A:LEU:HD21 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE1 | 1:19:A:LEU:HD22 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE1 | 1:19:A:LEU:HD23 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE2 | 1:19:A:LEU:HD11 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE2 | 1:19:A:LEU:HD12 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE2 | 1:19:A:LEU:HD13 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE2 | 1:19:A:LEU:HD21 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE2 | 1:19:A:LEU:HD22 | 40 | 0.12 |
| (1,959) | 1:18:A:PHE:HE2 | 1:19:A:LEU:HD23 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD11 | 1:18:A:PHE:HE1 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD11 | 1:18:A:PHE:HE2 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD12 | 1:18:A:PHE:HE1 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD12 | 1:18:A:PHE:HE2 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD13 | 1:18:A:PHE:HE1 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD13 | 1:18:A:PHE:HE2 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD21 | 1:18:A:PHE:HE1 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD21 | 1:18:A:PHE:HE2 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD22 | 1:18:A:PHE:HE1 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD22 | 1:18:A:PHE:HE2 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD23 | 1:18:A:PHE:HE1 | 40 | 0.12 |
| (1,955) | 1:19:A:LEU:HD23 | 1:18:A:PHE:HE2 | 40 | 0.12 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 17 | 0.12 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 17 | 0.12 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 34 | 0.12 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 34 | 0.12 |
| (1,405) | 1:23:A:PHE:HE1 | 1:23:A:PHE:H | 46 | 0.12 |
| (1,405) | 1:23:A:PHE:HE2 | 1:23:A:PHE:H | 46 | 0.12 |
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE1 | 46 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE2 | 46 | 0.12 |
| (2,17) | 1:22:A:GLY:O | 1:26:A:PHE:H | 41 | 0.11 |
| (2,14) | 1:19:A:LEU:O | 1:23:A:PHE:N | 48 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG11 | 25 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG12 | 25 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG13 | 25 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG21 | 25 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG22 | 25 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG23 | 25 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG11 | 29 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG12 | 29 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG13 | 29 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG21 | 29 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG22 | 29 | 0.11 |
| (1,1860) | 1:3:A:HIS:HD2 | 1:8:A:VAL:HG23 | 29 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG11 | 1:3:A:HIS:HD2 | 25 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG12 | 1:3:A:HIS:HD2 | 25 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG13 | 1:3:A:HIS:HD2 | 25 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG21 | 1:3:A:HIS:HD2 | 25 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG22 | 1:3:A:HIS:HD2 | 25 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG23 | 1:3:A:HIS:HD2 | 25 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG11 | 1:3:A:HIS:HD2 | 29 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG12 | 1:3:A:HIS:HD2 | 29 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG13 | 1:3:A:HIS:HD2 | 29 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG21 | 1:3:A:HIS:HD2 | 29 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG22 | 1:3:A:HIS:HD2 | 29 | 0.11 |
| (1,1854) | 1:8:A:VAL:HG23 | 1:3:A:HIS:HD2 | 29 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 5 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 5 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 9 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 9 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 17 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 17 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 19 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 19 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 29 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 29 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 30 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 30 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 31 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 31 | 0.11 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 35 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 35 | 0.11 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 37 | 0.11 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 37 | 0.11 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 49 | 0.11 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 49 | 0.11 |
| (1,1809) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HA | 17 | 0.11 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 44 | 0.11 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 48 | 0.11 |
| (1,1799) | 1:27:A:LYS:HG3 | 1:23:A:PHE:HD1 | 45 | 0.11 |
| (1,1799) | 1:27:A:LYS:HG3 | 1:23:A:PHE:HD2 | 45 | 0.11 |
| (1,1798) | 1:20:A:ALA:H | 1:22:A:GLY:HA2 | 35 | 0.11 |
| (1,1798) | 1:20:A:ALA:H | 1:22:A:GLY:HA3 | 35 | 0.11 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 25 | 0.11 |
| (1,1789) | 1:17:A:THR:HB | 1:16:A:LEU:H | 22 | 0.11 |
| (1,1789) | 1:17:A:THR:HB | 1:16:A:LEU:H | 32 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG11 | 36 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG12 | 36 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG13 | 36 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG21 | 36 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG22 | 36 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG23 | 36 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG11 | 37 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG12 | 37 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG13 | 37 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG21 | 37 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG22 | 37 | 0.11 |
| (1,1772) | 1:5:A:ILE:HG13 | 1:8:A:VAL:HG23 | 37 | 0.11 |
| (1,1745) | 1:25:A:LEU:HD11 | 1:24:A:TRP:HE3 | 16 | 0.11 |
| (1,1722) | 1:25:A:LEU:HD13 | 1:21:A:PHE:HD1 | 34 | 0.11 |
| (1,1722) | 1:25:A:LEU:HD13 | 1:21:A:PHE:HD2 | 34 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 22 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 22 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 22 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 22 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 22 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 22 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD11 | 48 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD12 | 48 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD13 | 48 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD21 | 48 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD22 | 48 | 0.11 |
| (1,1715) | 1:26:A:PHE:HZ | 1:25:A:LEU:HD23 | 48 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1674) | 1:29:A:LEU:H | 1:25:A:LEU:HG | 49 | 0.11 |
| (1,1672) | 1:25:A:LEU:HG | 1:29:A:LEU:H | 49 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 9 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 9 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 9 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 9 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 9 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 9 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 21 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 21 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 21 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 21 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 21 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 21 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 44 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 44 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 44 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 44 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 44 | 0.11 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 44 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 9 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 9 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 9 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 9 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 9 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 9 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 21 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 21 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 21 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 21 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 21 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 21 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 44 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 44 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 44 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 44 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 44 | 0.11 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 44 | 0.11 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 30 | 0.11 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 30 | 0.11 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 42 | 0.11 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 42 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ1 | 47 | 0.11 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ2 | 47 | 0.11 |
| (1,1126) | 1:28:A:TYR:H | 1:27:A:LYS:HZ3 | 47 | 0.11 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 43 | 0.11 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 43 | 0.11 |
| (1,405) | 1:23:A:PHE:HE1 | 1:23:A:PHE:H | 39 | 0.11 |
| (1,405) | 1:23:A:PHE:HE2 | 1:23:A:PHE:H | 39 | 0.11 |
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE1 | 39 | 0.11 |
| (1,404) | 1:23:A:PHE:H | 1:23:A:PHE:HE2 | 39 | 0.11 |
| (2,17) | 1:22:A:GLY:O | 1:26:A:PHE:H | 48 | 0.1 |
| (2,8) | 1:14:A:ALA:O | 1:18:A:PHE:N | 40 | 0.1 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 16 | 0.1 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 16 | 0.1 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 18 | 0.1 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 18 | 0.1 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE1 | 47 | 0.1 |
| (1,1836) | 1:19:A:LEU:H | 1:18:A:PHE:HE2 | 47 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 1 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 1 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 2 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 2 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 3 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 3 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 4 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 4 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 36 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 36 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE1 | 38 | 0.1 |
| (1,1821) | 1:25:A:LEU:HG | 1:28:A:TYR:HE2 | 38 | 0.1 |
| (1,1802) | 1:9:A:ILE:HA | 1:12:A:LEU:HG | 15 | 0.1 |
| (1,1790) | 1:22:A:GLY:HA3 | 1:19:A:LEU:H | 2 | 0.1 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD2 | 39 | 0.1 |
| (1,1701) | 1:22:A:GLY:HA2 | 1:27:A:LYS:HD3 | 39 | 0.1 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD2 | 39 | 0.1 |
| (1,1701) | 1:22:A:GLY:HA3 | 1:27:A:LYS:HD3 | 39 | 0.1 |
| (1,1610) | 1:19:A:LEU:HG | 1:15:A:LEU:HG | 40 | 0.1 |
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD1 | 46 | 0.1 |
| (1,1504) | 1:29:A:LEU:HB2 | 1:26:A:PHE:HD2 | 46 | 0.1 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD1 | 46 | 0.1 |
| (1,1504) | 1:29:A:LEU:HB3 | 1:26:A:PHE:HD2 | 46 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 7 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 7 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 7 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 7 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 7 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 7 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB2 | 24 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB1 | 1:7:A:GLU:HB3 | 24 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB2 | 24 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB2 | 1:7:A:GLU:HB3 | 24 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB2 | 24 | 0.1 |
| (1,1353) | 1:10:A:ALA:HB3 | 1:7:A:GLU:HB3 | 24 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 7 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 7 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 7 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 7 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 7 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 7 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB1 | 24 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB2 | 24 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB2 | 1:10:A:ALA:HB3 | 24 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB1 | 24 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB2 | 24 | 0.1 |
| (1,1352) | 1:7:A:GLU:HB3 | 1:10:A:ALA:HB3 | 24 | 0.1 |
| (1,1286) | 1:7:A:GLU:HB2 | 1:4:A:THR:H | 36 | 0.1 |
| (1,1286) | 1:7:A:GLU:HB3 | 1:4:A:THR:H | 36 | 0.1 |
| (1,1273) | 1:31:A:LYS:HD2 | 1:29:A:LEU:HA | 32 | 0.1 |
| (1,1273) | 1:31:A:LYS:HD3 | 1:29:A:LEU:HA | 32 | 0.1 |
| (1,1179) | 1:5:A:ILE:H | 1:3:A:HIS:HE1 | 19 | 0.1 |
| (1,1085) | 1:26:A:PHE:HD1 | 1:27:A:LYS:HG2 | 44 | 0.1 |
| (1,1085) | 1:26:A:PHE:HD1 | 1:27:A:LYS:HG3 | 44 | 0.1 |
| (1,1085) | 1:26:A:PHE:HD2 | 1:27:A:LYS:HG2 | 44 | 0.1 |
| (1,1085) | 1:26:A:PHE:HD2 | 1:27:A:LYS:HG3 | 44 | 0.1 |
| (1,1079) | 1:27:A:LYS:HG2 | 1:26:A:PHE:HD1 | 44 | 0.1 |
| (1,1079) | 1:27:A:LYS:HG2 | 1:26:A:PHE:HD2 | 44 | 0.1 |
| (1,1079) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HD1 | 44 | 0.1 |
| (1,1079) | 1:27:A:LYS:HG3 | 1:26:A:PHE:HD2 | 44 | 0.1 |
| (1,602) | 1:29:A:LEU:HD11 | 1:29:A:LEU:HA | 47 | 0.1 |
| (1,602) | 1:29:A:LEU:HD12 | 1:29:A:LEU:HA | 47 | 0.1 |
| (1,602) | 1:29:A:LEU:HD13 | 1:29:A:LEU:HA | 47 | 0.1 |
| (1,602) | 1:29:A:LEU:HD21 | 1:29:A:LEU:HA | 47 | 0.1 |
| (1,602) | 1:29:A:LEU:HD22 | 1:29:A:LEU:HA | 47 | 0.1 |
| (1,602) | 1:29:A:LEU:HD23 | 1:29:A:LEU:HA | 47 | 0.1 |
| (1,601) | 1:29:A:LEU:HA | 1:29:A:LEU:HD11 | 47 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,601) | 1:29:A:LEU:HA | 1:29:A:LEU:HD12 | 47 | 0.1 |
| (1,601) | 1:29:A:LEU:HA | 1:29:A:LEU:HD13 | 47 | 0.1 |
| (1,601) | 1:29:A:LEU:HA | 1:29:A:LEU:HD21 | 47 | 0.1 |
| (1,601) | 1:29:A:LEU:HA | 1:29:A:LEU:HD22 | 47 | 0.1 |
| (1,601) | 1:29:A:LEU:HA | 1:29:A:LEU:HD23 | 47 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 10 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 10 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 11 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 11 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 13 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 13 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 26 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 26 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 27 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 27 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD1 | 31 | 0.1 |
| (1,575) | 1:28:A:TYR:HA | 1:28:A:TYR:HD2 | 31 | 0.1 |
| (1,98) | 1:6:A:TRP:HD1 | 1:6:A:TRP:HE3 | 6 | 0.1 |
| (1,98) | 1:6:A:TRP:HD1 | 1:6:A:TRP:HE3 | 37 | 0.1 |
| (1,98) | 1:6:A:TRP:HD1 | 1:6:A:TRP:HE3 | 38 | 0.1 |

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

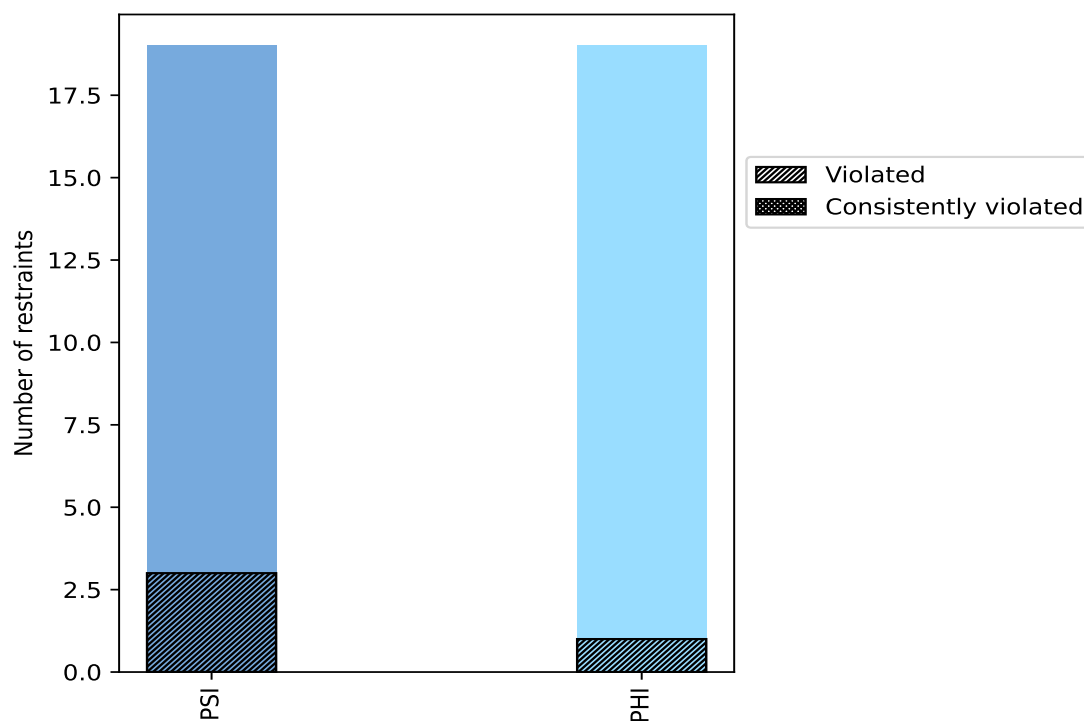
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PSI | 19 | 50.0 | 3 | 15.8 | 7.9 | 0 | 0.0 | 0.0 |
| PHI | 19 | 50.0 | 1 | 5.3 | 2.6 | 0 | 0.0 | 0.0 |
| Total | 38 | 100.0 | 4 | 10.5 | 10.5 | 0 | 0.0 | 0.0 |

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

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



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

10.2 Dihedral-angle violation statistics for each model [i](#)

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

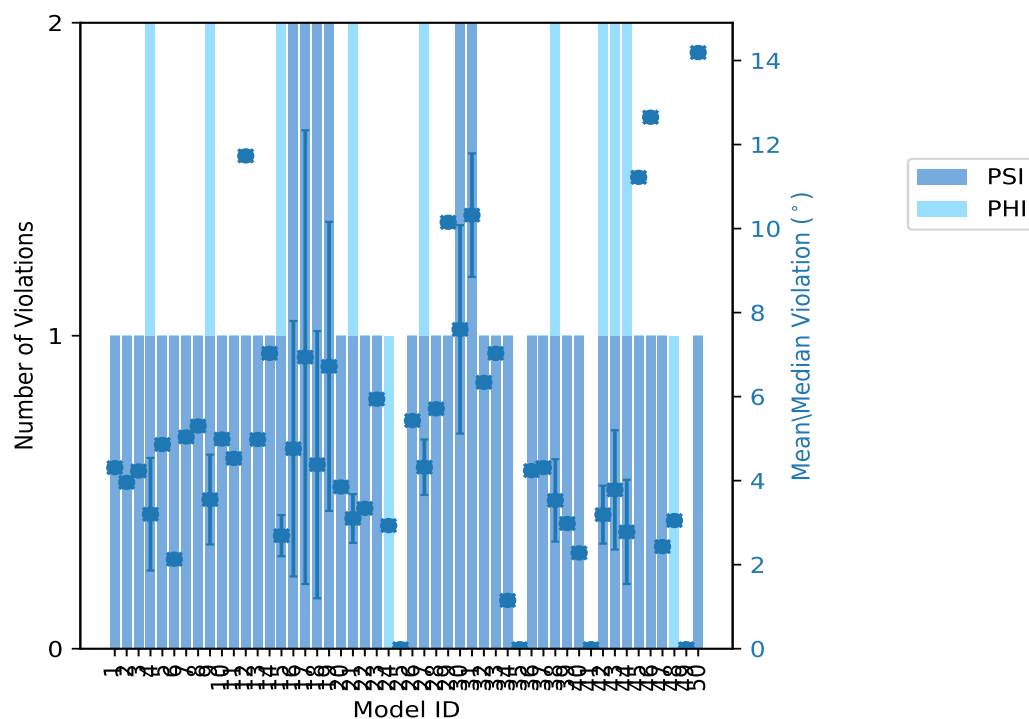
| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PSI | PHI | Total | | | | |
| 1 | 1 | 0 | 1 | 4.31 | 4.31 | 0.0 | 4.31 |
| 2 | 1 | 0 | 1 | 3.96 | 3.96 | 0.0 | 3.96 |
| 3 | 1 | 0 | 1 | 4.23 | 4.23 | 0.0 | 4.23 |
| 4 | 1 | 1 | 2 | 3.2 | 4.54 | 1.34 | 3.2 |
| 5 | 1 | 0 | 1 | 4.86 | 4.86 | 0.0 | 4.86 |
| 6 | 1 | 0 | 1 | 2.13 | 2.13 | 0.0 | 2.13 |
| 7 | 1 | 0 | 1 | 5.04 | 5.04 | 0.0 | 5.04 |
| 8 | 1 | 0 | 1 | 5.3 | 5.3 | 0.0 | 5.3 |
| 9 | 1 | 1 | 2 | 3.55 | 4.62 | 1.07 | 3.55 |
| 10 | 1 | 0 | 1 | 4.99 | 4.99 | 0.0 | 4.99 |
| 11 | 1 | 0 | 1 | 4.53 | 4.53 | 0.0 | 4.53 |
| 12 | 1 | 0 | 1 | 11.73 | 11.73 | 0.0 | 11.73 |
| 13 | 1 | 0 | 1 | 4.98 | 4.98 | 0.0 | 4.98 |
| 14 | 1 | 0 | 1 | 7.03 | 7.03 | 0.0 | 7.03 |
| 15 | 1 | 1 | 2 | 2.69 | 3.18 | 0.49 | 2.69 |
| 16 | 2 | 0 | 2 | 4.76 | 7.8 | 3.04 | 4.76 |
| 17 | 2 | 0 | 2 | 6.94 | 12.34 | 5.4 | 6.94 |
| 18 | 2 | 0 | 2 | 4.38 | 7.57 | 3.18 | 4.38 |
| 19 | 2 | 0 | 2 | 6.72 | 10.16 | 3.44 | 6.72 |
| 20 | 1 | 0 | 1 | 3.85 | 3.85 | 0.0 | 3.85 |
| 21 | 1 | 1 | 2 | 3.1 | 3.69 | 0.58 | 3.1 |
| 22 | 1 | 0 | 1 | 3.34 | 3.34 | 0.0 | 3.34 |
| 23 | 1 | 0 | 1 | 5.94 | 5.94 | 0.0 | 5.94 |
| 24 | 0 | 1 | 1 | 2.93 | 2.93 | 0.0 | 2.93 |
| 25 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 26 | 1 | 0 | 1 | 5.43 | 5.43 | 0.0 | 5.43 |
| 27 | 1 | 1 | 2 | 4.32 | 4.98 | 0.66 | 4.32 |
| 28 | 1 | 0 | 1 | 5.71 | 5.71 | 0.0 | 5.71 |
| 29 | 1 | 0 | 1 | 10.15 | 10.15 | 0.0 | 10.15 |
| 30 | 2 | 0 | 2 | 7.6 | 10.09 | 2.48 | 7.6 |
| 31 | 2 | 0 | 2 | 10.32 | 11.79 | 1.47 | 10.32 |
| 32 | 1 | 0 | 1 | 6.34 | 6.34 | 0.0 | 6.34 |
| 33 | 1 | 0 | 1 | 7.03 | 7.03 | 0.0 | 7.03 |
| 34 | 1 | 0 | 1 | 1.15 | 1.15 | 0.0 | 1.15 |
| 35 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 36 | 1 | 0 | 1 | 4.24 | 4.24 | 0.0 | 4.24 |
| 37 | 1 | 0 | 1 | 4.31 | 4.31 | 0.0 | 4.31 |
| 38 | 1 | 1 | 2 | 3.53 | 4.51 | 0.98 | 3.53 |

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| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PSI | PHI | Total | | | | |
| 39 | 1 | 0 | 1 | 2.98 | 2.98 | 0.0 | 2.98 |
| 40 | 1 | 0 | 1 | 2.28 | 2.28 | 0.0 | 2.28 |
| 41 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 42 | 1 | 1 | 2 | 3.19 | 3.88 | 0.69 | 3.19 |
| 43 | 1 | 1 | 2 | 3.78 | 5.2 | 1.42 | 3.78 |
| 44 | 1 | 1 | 2 | 2.78 | 4.02 | 1.24 | 2.78 |
| 45 | 1 | 0 | 1 | 11.22 | 11.22 | 0.0 | 11.22 |
| 46 | 1 | 0 | 1 | 12.65 | 12.65 | 0.0 | 12.65 |
| 47 | 1 | 0 | 1 | 2.43 | 2.43 | 0.0 | 2.43 |
| 48 | 0 | 1 | 1 | 3.05 | 3.05 | 0.0 | 3.05 |
| 49 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 50 | 1 | 0 | 1 | 14.19 | 14.19 | 0.0 | 14.19 |

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 1 | 2.0 |
| 0 | 0 | 0 | 2 | 4.0 |
| 0 | 0 | 0 | 3 | 6.0 |
| 0 | 0 | 0 | 4 | 8.0 |
| 0 | 0 | 0 | 5 | 10.0 |
| 1 | 0 | 1 | 6 | 12.0 |
| 0 | 0 | 0 | 7 | 14.0 |
| 0 | 0 | 0 | 8 | 16.0 |
| 0 | 0 | 0 | 9 | 18.0 |
| 1 | 0 | 1 | 10 | 20.0 |
| 0 | 1 | 1 | 11 | 22.0 |
| 0 | 0 | 0 | 12 | 24.0 |
| 0 | 0 | 0 | 13 | 26.0 |
| 0 | 0 | 0 | 14 | 28.0 |
| 0 | 0 | 0 | 15 | 30.0 |
| 0 | 0 | 0 | 16 | 32.0 |
| 0 | 0 | 0 | 17 | 34.0 |
| 0 | 0 | 0 | 18 | 36.0 |
| 0 | 0 | 0 | 19 | 38.0 |
| 0 | 0 | 0 | 20 | 40.0 |
| 0 | 0 | 0 | 21 | 42.0 |
| 0 | 0 | 0 | 22 | 44.0 |
| 0 | 0 | 0 | 23 | 46.0 |
| 0 | 0 | 0 | 24 | 48.0 |
| 0 | 0 | 0 | 25 | 50.0 |
| 0 | 0 | 0 | 26 | 52.0 |
| 0 | 0 | 0 | 27 | 54.0 |
| 0 | 0 | 0 | 28 | 56.0 |
| 0 | 0 | 0 | 29 | 58.0 |
| 0 | 0 | 0 | 30 | 60.0 |
| 0 | 0 | 0 | 31 | 62.0 |
| 0 | 0 | 0 | 32 | 64.0 |
| 0 | 0 | 0 | 33 | 66.0 |
| 1 | 0 | 1 | 34 | 68.0 |
| 0 | 0 | 0 | 35 | 70.0 |
| 0 | 0 | 0 | 36 | 72.0 |
| 0 | 0 | 0 | 37 | 74.0 |

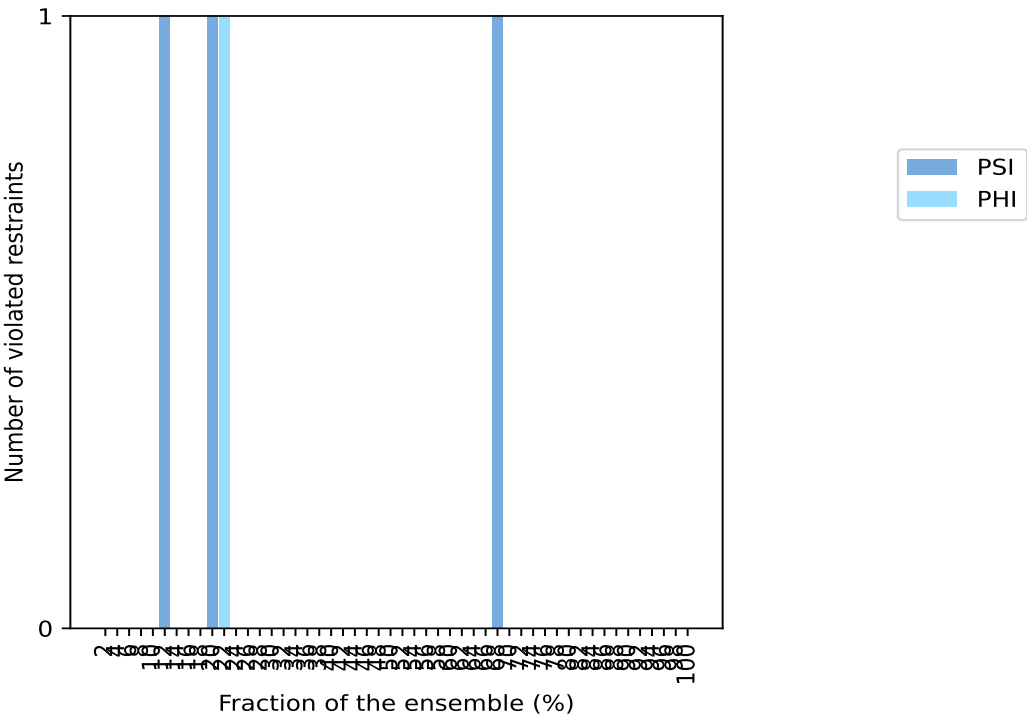
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 38 | 76.0 |
| 0 | 0 | 0 | 39 | 78.0 |
| 0 | 0 | 0 | 40 | 80.0 |
| 0 | 0 | 0 | 41 | 82.0 |
| 0 | 0 | 0 | 42 | 84.0 |
| 0 | 0 | 0 | 43 | 86.0 |
| 0 | 0 | 0 | 44 | 88.0 |
| 0 | 0 | 0 | 45 | 90.0 |
| 0 | 0 | 0 | 46 | 92.0 |
| 0 | 0 | 0 | 47 | 94.0 |
| 0 | 0 | 0 | 48 | 96.0 |
| 0 | 0 | 0 | 49 | 98.0 |
| 0 | 0 | 0 | 50 | 100.0 |

¹ Number of models with violations

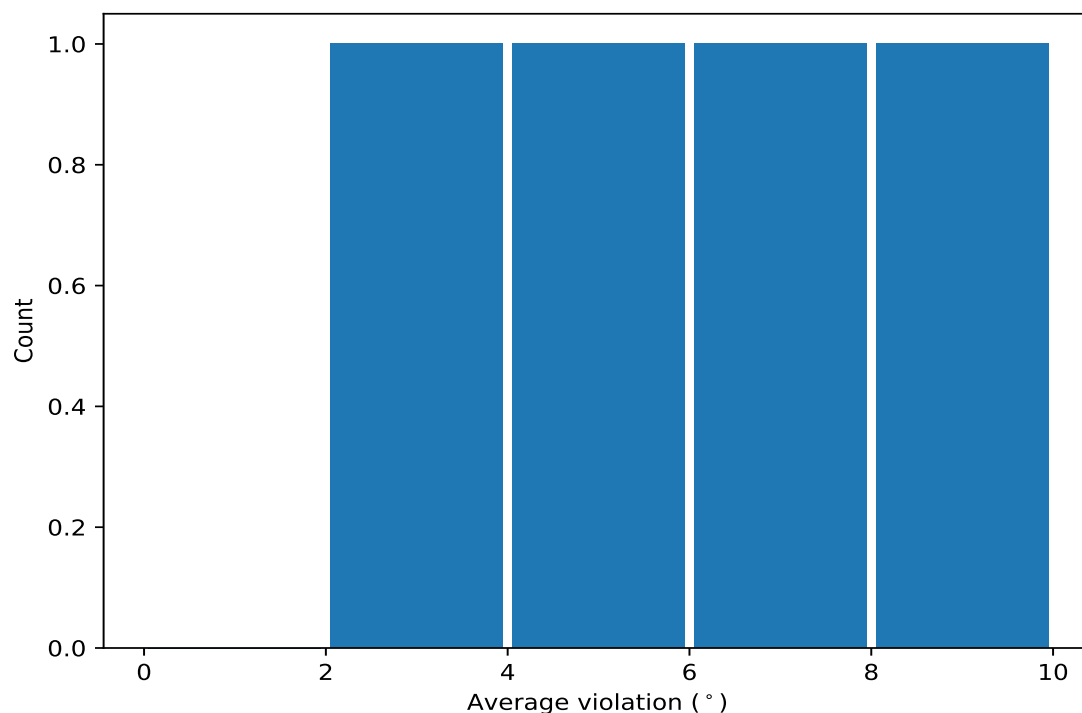
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

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

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



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

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

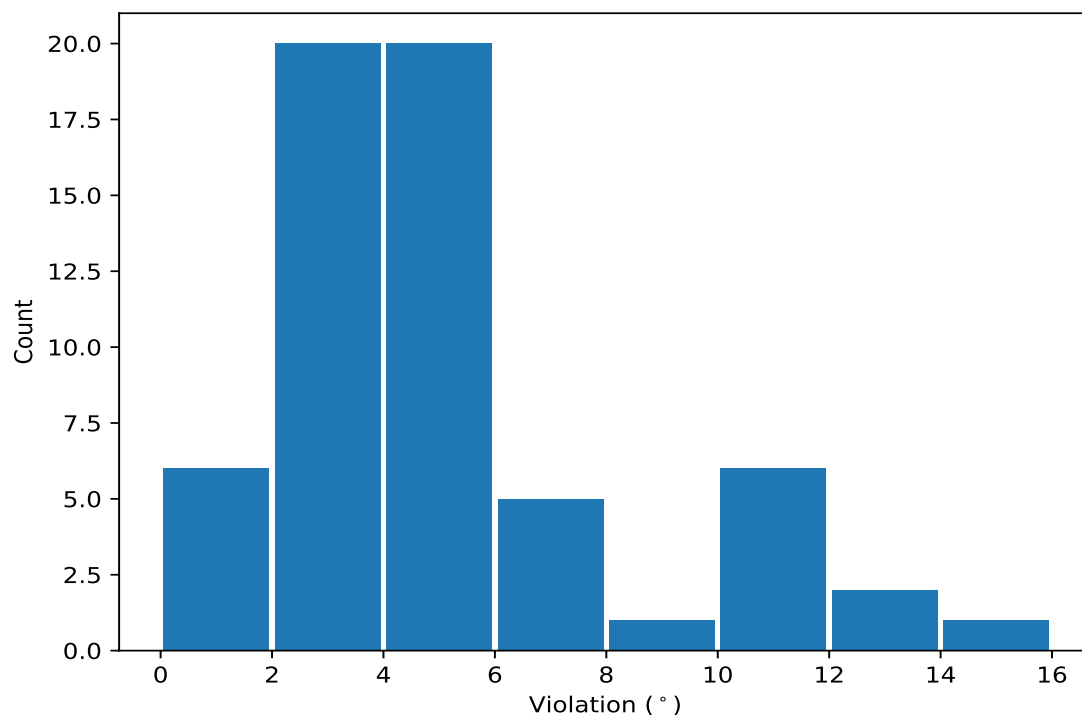
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 34 | 4.61 | 2.16 | 4.52 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 11 | 2.51 | 0.55 | 2.5 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 10 | 7.49 | 4.58 | 8.17 |
| (1,30) | 1:23:A:PHE:N | 1:23:A:PHE:CA | 1:23:A:PHE:C | 1:24:A:TRP:N | 6 | 9.1 | 1.1 | 9.46 |

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 50 | 14.19 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 46 | 12.65 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 17 | 12.34 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 31 | 11.79 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 12 | 11.73 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 45 | 11.22 |
| (1,30) | 1:23:A:PHE:N | 1:23:A:PHE:CA | 1:23:A:PHE:C | 1:24:A:TRP:N | 19 | 10.16 |
| (1,30) | 1:23:A:PHE:N | 1:23:A:PHE:CA | 1:23:A:PHE:C | 1:24:A:TRP:N | 29 | 10.15 |
| (1,30) | 1:23:A:PHE:N | 1:23:A:PHE:CA | 1:23:A:PHE:C | 1:24:A:TRP:N | 30 | 10.09 |
| (1,30) | 1:23:A:PHE:N | 1:23:A:PHE:CA | 1:23:A:PHE:C | 1:24:A:TRP:N | 31 | 8.84 |
| (1,30) | 1:23:A:PHE:N | 1:23:A:PHE:CA | 1:23:A:PHE:C | 1:24:A:TRP:N | 16 | 7.8 |
| (1,30) | 1:23:A:PHE:N | 1:23:A:PHE:CA | 1:23:A:PHE:C | 1:24:A:TRP:N | 18 | 7.57 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 14 | 7.03 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 33 | 7.03 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 32 | 6.34 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 23 | 5.94 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 28 | 5.71 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 26 | 5.43 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 8 | 5.3 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 43 | 5.2 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 30 | 5.12 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 7 | 5.04 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 10 | 4.99 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 13 | 4.98 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 27 | 4.98 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 5 | 4.86 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 9 | 4.62 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 4 | 4.54 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 11 | 4.53 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 38 | 4.51 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 1 | 4.31 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 37 | 4.31 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 36 | 4.24 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 3 | 4.23 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 44 | 4.02 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 2 | 3.96 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 42 | 3.88 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 20 | 3.85 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 21 | 3.69 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 27 | 3.66 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 22 | 3.34 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 19 | 3.27 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 15 | 3.18 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 48 | 3.05 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 39 | 2.98 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 24 | 2.93 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 38 | 2.55 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 21 | 2.52 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 42 | 2.5 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 9 | 2.48 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 47 | 2.43 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 43 | 2.37 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 40 | 2.28 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 15 | 2.2 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 6 | 2.13 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 4 | 1.85 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 16 | 1.71 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 17 | 1.53 |
| (1,17) | 1:16:A:LEU:C | 1:17:A:THR:N | 1:17:A:THR:CA | 1:17:A:THR:C | 44 | 1.53 |
| (1,38) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C | 1:28:A:TYR:N | 18 | 1.2 |
| (1,36) | 1:26:A:PHE:N | 1:26:A:PHE:CA | 1:26:A:PHE:C | 1:27:A:LYS:N | 34 | 1.15 |