



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 06:03 PM EST

PDB ID : 7DM4
BMRB ID : 50612
Title : Solution structure of ARID4B Tudor domain
Authors : Ren, J.; Yao, H.; Hu, W.; Perrett, S.; Feng, Y.; Gong, W.
Deposited on : 2020-12-02

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

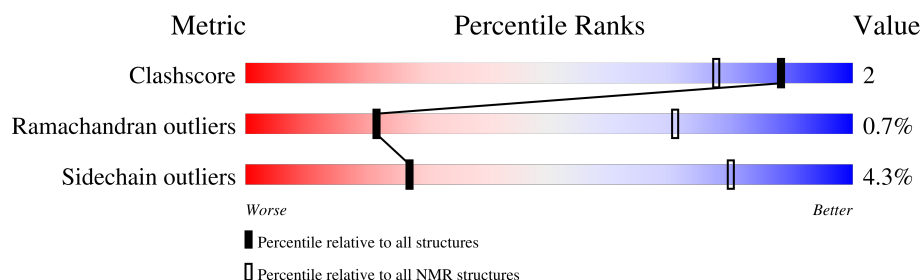
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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 | 151 | <div> <div style="width: 64%; background-color: green;"></div> <div style="width: 36%; background-color: cyan;"></div> </div> <div>64% . 36%</div> |

2 Ensemble composition and analysis

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

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|---------------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:9-A:33, A:87-A:109 (48) | 0.78 | 5 |
| 2 | A:36-A:84 (49) | 0.52 | 19 |

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2394 atoms, of which 1205 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called AT-rich interactive domain-containing protein 4B.

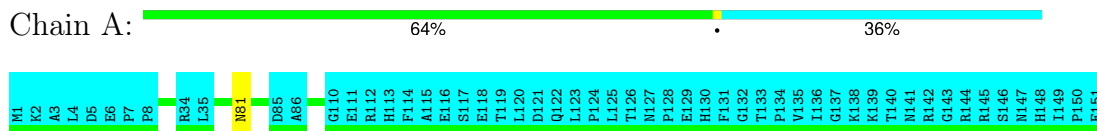
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1 | A | 151 | Total | C | H | N | O | S | 0 |
| | | | 2394 | 746 | 1205 | 212 | 228 | 3 | |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: AT-rich interactive domain-containing protein 4B

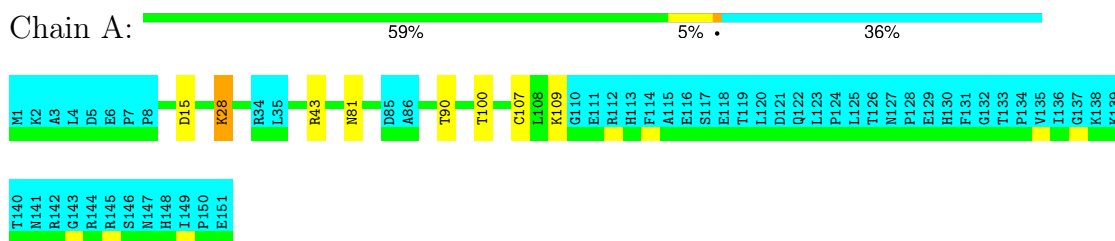


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

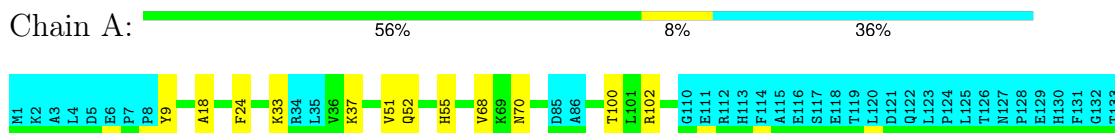
4.2.1 Score per residue for model 1

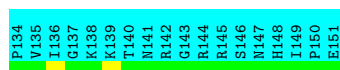
- Molecule 1: AT-rich interactive domain-containing protein 4B



4.2.2 Score per residue for model 2

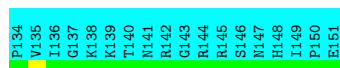
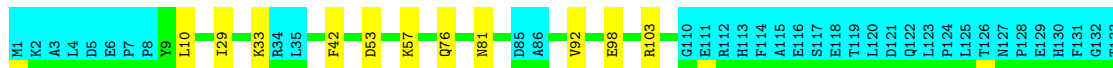
- Molecule 1: AT-rich interactive domain-containing protein 4B





4.2.3 Score per residue for model 3

- Molecule 1: AT-rich interactive domain-containing protein 4B



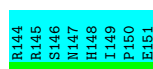
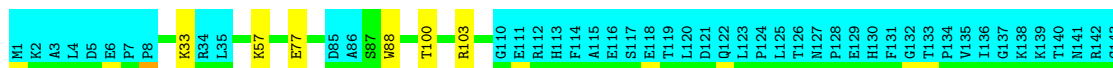
4.2.4 Score per residue for model 4

- Molecule 1: AT-rich interactive domain-containing protein 4B



4.2.5 Score per residue for model 5

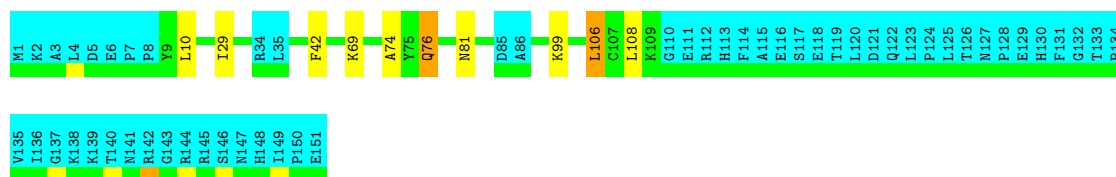
- Molecule 1: AT-rich interactive domain-containing protein 4B



4.2.6 Score per residue for model 6

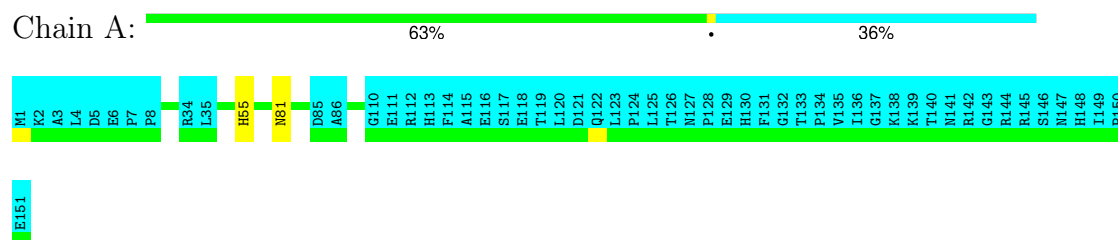
- Molecule 1: AT-rich interactive domain-containing protein 4B





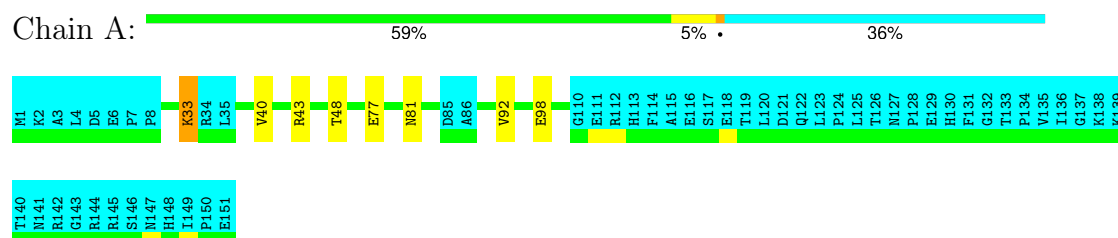
4.2.7 Score per residue for model 7

- Molecule 1: AT-rich interactive domain-containing protein 4B



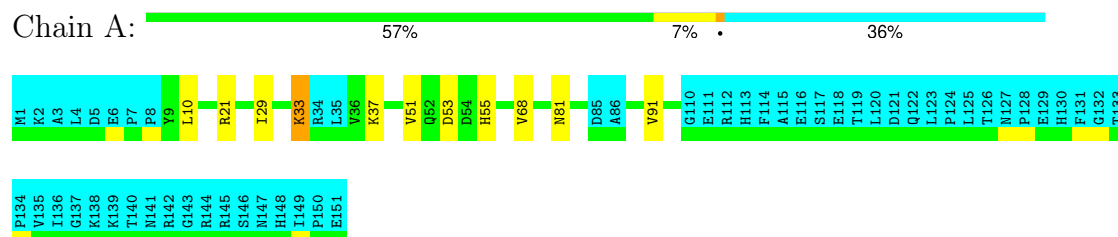
4.2.8 Score per residue for model 8

- Molecule 1: AT-rich interactive domain-containing protein 4B



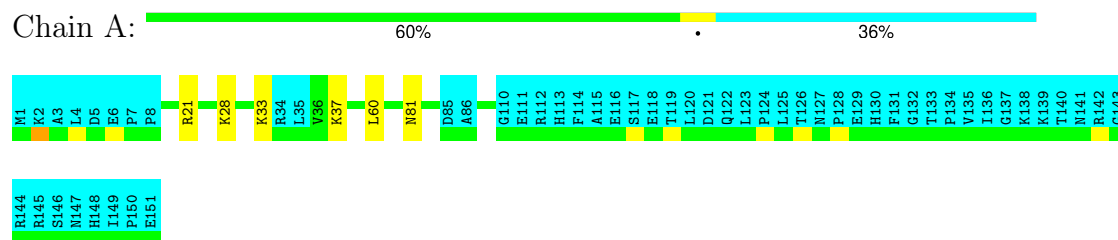
4.2.9 Score per residue for model 9

- Molecule 1: AT-rich interactive domain-containing protein 4B



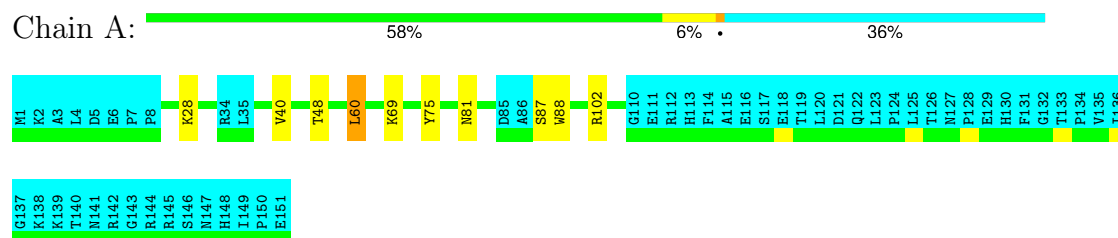
4.2.10 Score per residue for model 10

- Molecule 1: AT-rich interactive domain-containing protein 4B



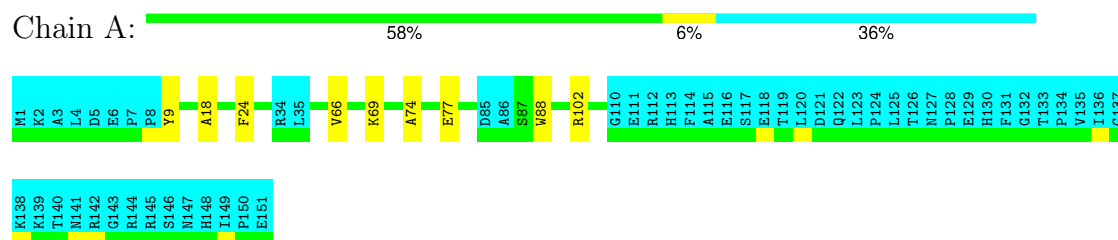
4.2.11 Score per residue for model 11

- Molecule 1: AT-rich interactive domain-containing protein 4B



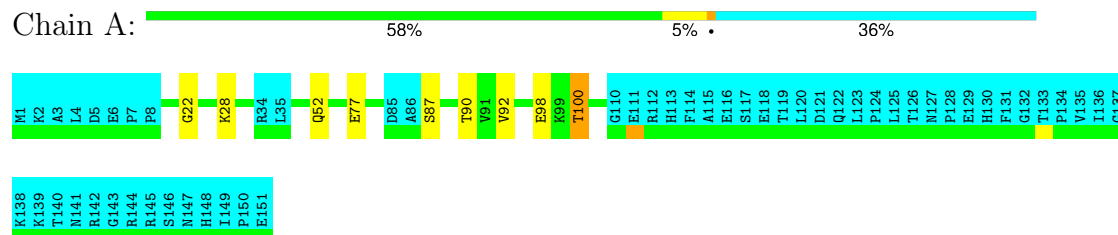
4.2.12 Score per residue for model 12

- Molecule 1: AT-rich interactive domain-containing protein 4B



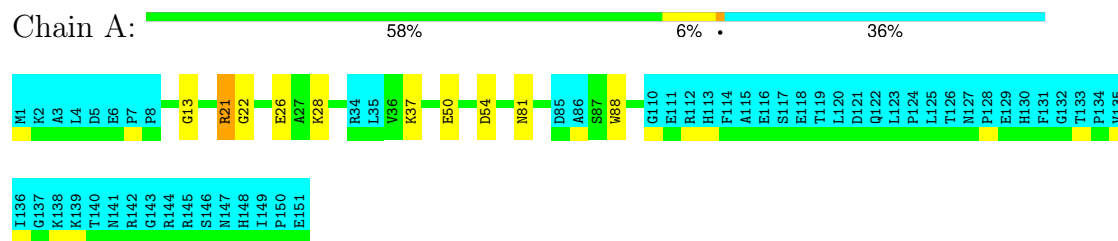
4.2.13 Score per residue for model 13

- Molecule 1: AT-rich interactive domain-containing protein 4B



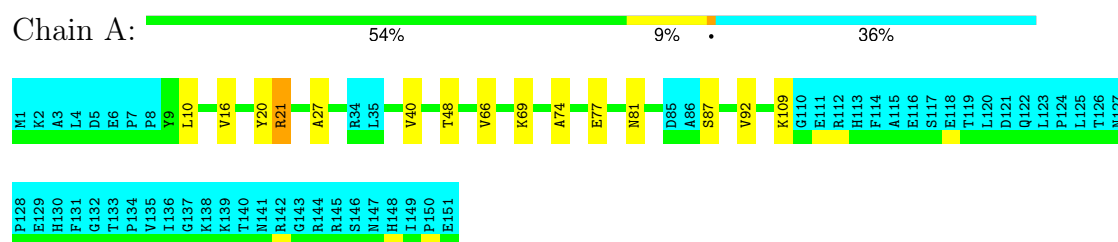
4.2.14 Score per residue for model 14

- Molecule 1: AT-rich interactive domain-containing protein 4B



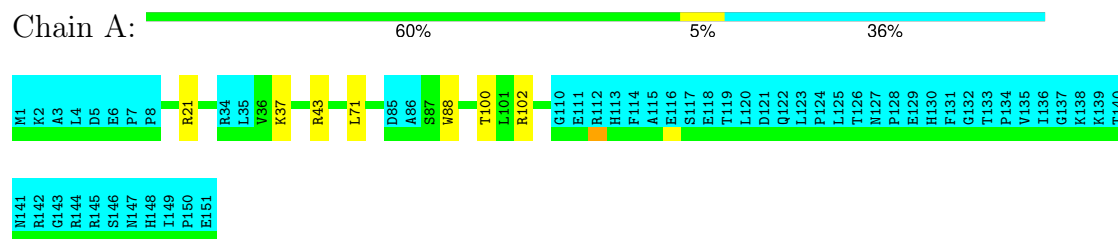
4.2.15 Score per residue for model 15

- Molecule 1: AT-rich interactive domain-containing protein 4B



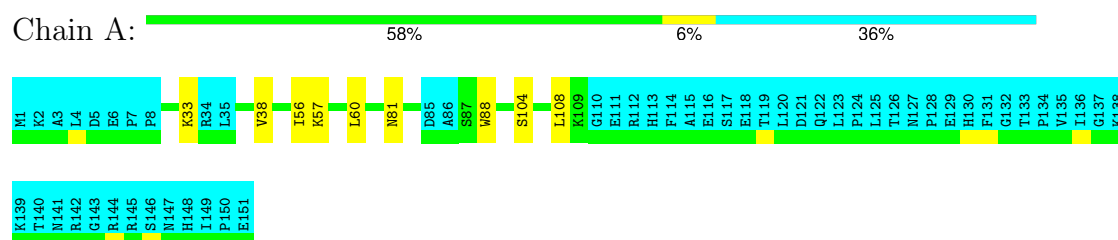
4.2.16 Score per residue for model 16

- Molecule 1: AT-rich interactive domain-containing protein 4B



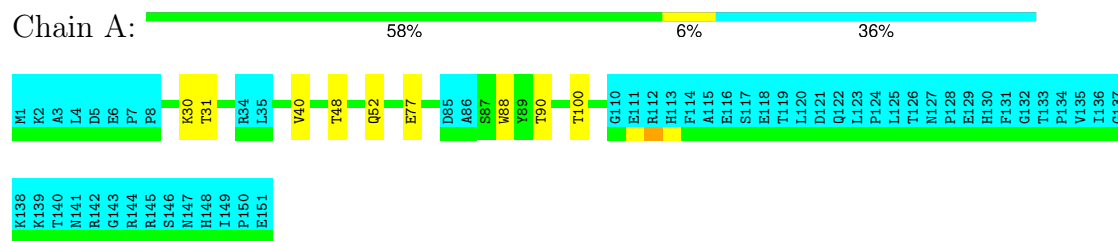
4.2.17 Score per residue for model 17

- Molecule 1: AT-rich interactive domain-containing protein 4B



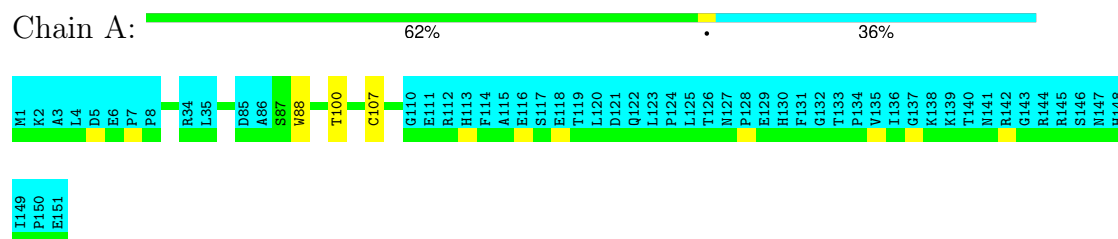
4.2.18 Score per residue for model 18

- Molecule 1: AT-rich interactive domain-containing protein 4B



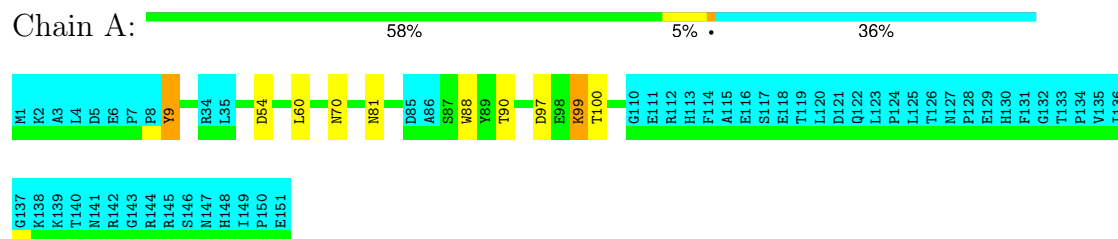
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: AT-rich interactive domain-containing protein 4B



4.2.20 Score per residue for model 20

- Molecule 1: AT-rich interactive domain-containing protein 4B



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1774 |
| Number of shifts mapped to atoms | 1774 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 90% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0.0±0.0 | 0.1±0.4 |
| All | All | 0 | 3 |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 43 | ARG | Sidechain | 3 |

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 | 759 | 781 | 779 | 3±2 |
| All | All | 15180 | 15620 | 15580 | 54 |

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 2.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:28:LYS:N | 1:A:28:LYS:HE2 | 0.60 | 2.11 | 1 | 1 |
| 1:A:92:VAL:HG22 | 1:A:98:GLU:HG2 | 0.55 | 1.79 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:88:TRP:HB3 | 1:A:100:THR:HB | 0.54 | 1.79 | 19 | 2 |
| 1:A:92:VAL:HG22 | 1:A:98:GLU:HG3 | 0.54 | 1.79 | 13 | 1 |
| 1:A:51:VAL:HB | 1:A:55:HIS:CE1 | 0.51 | 2.41 | 2 | 1 |
| 1:A:29:ILE:HD13 | 1:A:91:VAL:HG12 | 0.51 | 1.82 | 9 | 1 |
| 1:A:43:ARG:HA | 1:A:43:ARG:NE | 0.50 | 2.21 | 16 | 1 |
| 1:A:27:ALA:HA | 1:A:92:VAL:O | 0.50 | 2.06 | 15 | 1 |
| 1:A:40:VAL:O | 1:A:48:THR:HA | 0.50 | 2.06 | 15 | 4 |
| 1:A:69:LYS:HB2 | 1:A:75:TYR:CE2 | 0.49 | 2.42 | 11 | 1 |
| 1:A:88:TRP:CB | 1:A:100:THR:HB | 0.49 | 2.37 | 19 | 1 |
| 1:A:10:LEU:CD2 | 1:A:106:LEU:HD13 | 0.48 | 2.38 | 6 | 1 |
| 1:A:55:HIS:CD2 | 1:A:68:VAL:HG13 | 0.48 | 2.44 | 2 | 1 |
| 1:A:57:LYS:HD2 | 1:A:57:LYS:N | 0.48 | 2.24 | 3 | 1 |
| 1:A:88:TRP:HB3 | 1:A:100:THR:OG1 | 0.47 | 2.10 | 5 | 3 |
| 1:A:31:THR:HB | 1:A:90:THR:HB | 0.47 | 1.84 | 18 | 1 |
| 1:A:55:HIS:NE2 | 1:A:68:VAL:HG13 | 0.47 | 2.25 | 2 | 1 |
| 1:A:90:THR:HA | 1:A:100:THR:HA | 0.46 | 1.87 | 1 | 3 |
| 1:A:69:LYS:HA | 1:A:74:ALA:O | 0.46 | 2.11 | 15 | 3 |
| 1:A:30:LYS:HA | 1:A:30:LYS:HE2 | 0.46 | 1.88 | 18 | 1 |
| 1:A:18:ALA:O | 1:A:24:PHE:HA | 0.44 | 2.13 | 12 | 2 |
| 1:A:37:LYS:HA | 1:A:51:VAL:O | 0.44 | 2.13 | 9 | 1 |
| 1:A:15:ASP:O | 1:A:109:LYS:HB2 | 0.43 | 2.13 | 1 | 1 |
| 1:A:10:LEU:HD23 | 1:A:16:VAL:HG11 | 0.43 | 1.89 | 15 | 1 |
| 1:A:42:PHE:HB3 | 1:A:76:GLN:OE1 | 0.43 | 2.14 | 6 | 2 |
| 1:A:97:ASP:OD2 | 1:A:99:LYS:HE2 | 0.42 | 2.14 | 20 | 1 |
| 1:A:88:TRP:CD1 | 1:A:102:ARG:HG2 | 0.42 | 2.49 | 11 | 1 |
| 1:A:66:VAL:O | 1:A:77:GLU:HA | 0.42 | 2.14 | 15 | 2 |
| 1:A:21:ARG:HA | 1:A:21:ARG:NE | 0.42 | 2.30 | 14 | 1 |
| 1:A:60:LEU:H | 1:A:60:LEU:HD23 | 0.42 | 1.75 | 17 | 2 |
| 1:A:33:LYS:HE2 | 1:A:33:LYS:HA | 0.42 | 1.91 | 8 | 2 |
| 1:A:92:VAL:CG2 | 1:A:98:GLU:HG3 | 0.42 | 2.45 | 13 | 1 |
| 1:A:10:LEU:HD23 | 1:A:29:ILE:HD11 | 0.41 | 1.91 | 9 | 1 |
| 1:A:10:LEU:HB3 | 1:A:29:ILE:CD1 | 0.41 | 2.45 | 6 | 2 |
| 1:A:55:HIS:O | 1:A:68:VAL:HA | 0.41 | 2.15 | 9 | 1 |
| 1:A:37:LYS:HD3 | 1:A:50:GLU:CD | 0.41 | 2.36 | 14 | 1 |
| 1:A:92:VAL:HG13 | 1:A:98:GLU:HG2 | 0.40 | 1.94 | 8 | 1 |
| 1:A:38:VAL:HG11 | 1:A:56:ILE:HG13 | 0.40 | 1.94 | 17 | 1 |

6.3 Torsion angles

6.3.1 Protein backbone

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1 | A | 97/151 (64%) | 94±1 (97±1%) | 2±1 (2±1%) | 1±1 (1±1%) | 21 | 71 |
| All | All | 1940/3020 (64%) | 1882 (97%) | 45 (2%) | 13 (1%) | 21 | 71 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 21 | ARG | 4 |
| 1 | A | 9 | TYR | 3 |
| 1 | A | 87 | SER | 3 |
| 1 | A | 22 | GLY | 2 |
| 1 | A | 60 | LEU | 1 |

6.3.2 Protein sidechains

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1 | A | 84/131 (64%) | 80±2 (96±2%) | 4±2 (4±2%) | 27 | 80 |
| All | All | 1680/2620 (64%) | 1607 (96%) | 73 (4%) | 27 | 80 |

All 27 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 | 81 | ASN | 13 |
| 1 | A | 33 | LYS | 7 |
| 1 | A | 28 | LYS | 6 |
| 1 | A | 102 | ARG | 4 |
| 1 | A | 77 | GLU | 4 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 37 | LYS | 3 |
| 1 | A | 52 | GLN | 3 |
| 1 | A | 21 | ARG | 3 |
| 1 | A | 54 | ASP | 3 |
| 1 | A | 88 | TRP | 3 |
| 1 | A | 70 | ASN | 2 |
| 1 | A | 100 | THR | 2 |
| 1 | A | 53 | ASP | 2 |
| 1 | A | 57 | LYS | 2 |
| 1 | A | 99 | LYS | 2 |
| 1 | A | 108 | LEU | 2 |
| 1 | A | 60 | LEU | 2 |
| 1 | A | 103 | ARG | 1 |
| 1 | A | 76 | GLN | 1 |
| 1 | A | 106 | LEU | 1 |
| 1 | A | 55 | HIS | 1 |
| 1 | A | 26 | GLU | 1 |
| 1 | A | 20 | TYR | 1 |
| 1 | A | 109 | LYS | 1 |
| 1 | A | 71 | LEU | 1 |
| 1 | A | 104 | SER | 1 |
| 1 | A | 9 | TYR | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 90% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_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 | 1774 |
| Number of shifts mapped to atoms | 1774 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 149 | 0.01 ± 0.11 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 139 | 0.08 ± 0.09 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 146 | 0.14 ± 0.05 | None needed (< 0.5 ppm) |
| ^{15}N | 141 | -0.39 ± 0.39 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1185 atoms were assigned a chemical shift out of a possible 1324. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone | 488/489 (100%) | 199/199 (100%) | 193/194 (99%) | 96/96 (100%) |
| Sidechain | 659/741 (89%) | 448/481 (93%) | 207/232 (89%) | 4/28 (14%) |

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| | Total | ^1H | ^{13}C | ^{15}N |
|----------|-----------------|---------------|-----------------|-----------------|
| Aromatic | 38/94 (40%) | 19/45 (42%) | 18/44 (41%) | 1/5 (20%) |
| Overall | 1185/1324 (90%) | 666/725 (92%) | 418/470 (89%) | 101/129 (78%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1774 atoms were assigned a chemical shift out of a possible 2066. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 736/751 (98%) | 300/305 (98%) | 295/302 (98%) | 141/144 (98%) |
| Sidechain | 1000/1177 (85%) | 676/760 (89%) | 316/367 (86%) | 8/50 (16%) |
| Aromatic | 38/138 (28%) | 19/67 (28%) | 18/60 (30%) | 1/11 (9%) |
| Overall | 1774/2066 (86%) | 995/1132 (88%) | 629/729 (86%) | 150/205 (73%) |

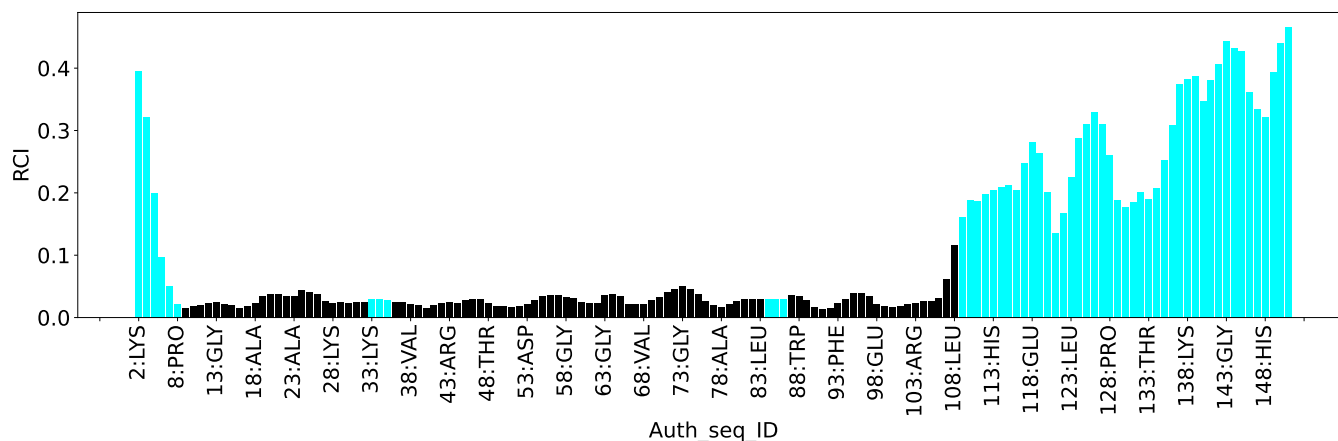
7.1.4 Statistically unusual chemical shifts [i](#)

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 | 3790 |
| Intra-residue ($ i-j =0$) | 1231 |
| Sequential ($ i-j =1$) | 864 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 397 |
| Long range ($ i-j \geq 5$) | 1224 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 74 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 170 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 26.2 |
| Number of long range restraints per residue ¹ | 8.5 |

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) | 28.9 | 0.2 |
| 0.2-0.5 (Medium) | 38.5 | 0.5 |
| >0.5 (Large) | 12.7 | 1.95 |

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) | 7.9 | 3.8 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

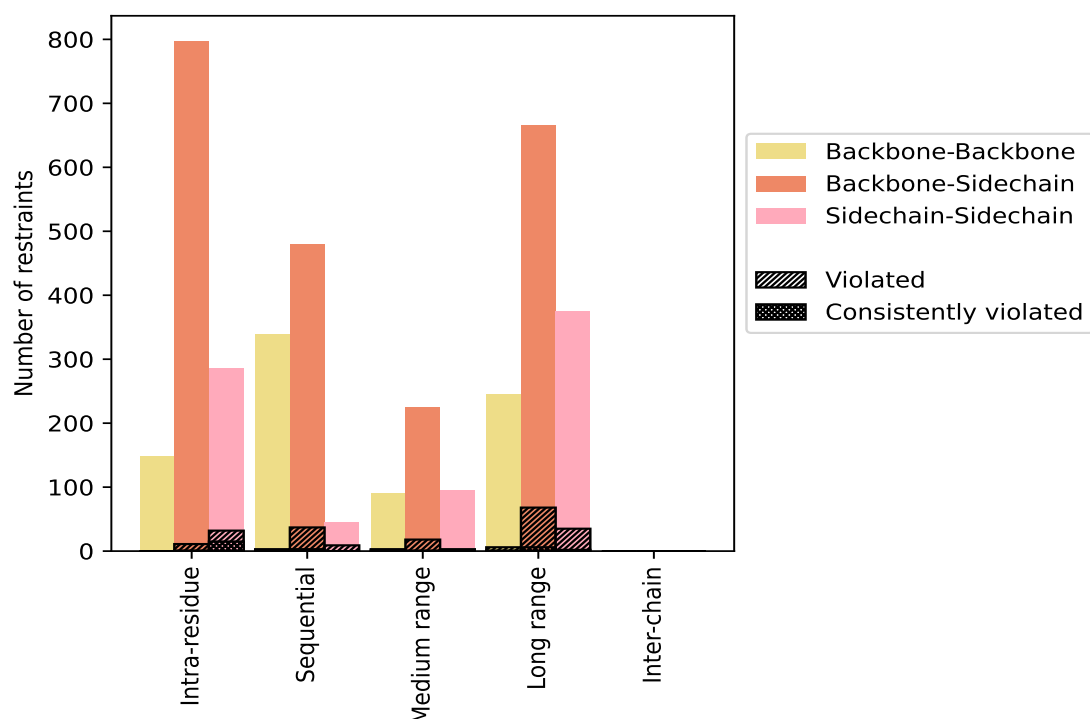
9.1 Summary of distance violations ⓘ

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

| Restraints type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 1231 | 32.5 | 43 | 3.5 | 1.1 | 16 | 1.3 | 0.4 |
| Backbone-Backbone | 148 | 3.9 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 797 | 21.0 | 11 | 1.4 | 0.3 | 1 | 0.1 | 0.0 |
| Sidechain-Sidechain | 286 | 7.5 | 32 | 11.2 | 0.8 | 15 | 5.2 | 0.4 |
| Sequential ($i-j =1$) | 864 | 22.8 | 49 | 5.7 | 1.3 | 3 | 0.3 | 0.1 |
| Backbone-Backbone | 339 | 8.9 | 3 | 0.9 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 480 | 12.7 | 37 | 7.7 | 1.0 | 3 | 0.6 | 0.1 |
| Sidechain-Sidechain | 45 | 1.2 | 9 | 20.0 | 0.2 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 397 | 10.5 | 24 | 6.0 | 0.6 | 2 | 0.5 | 0.1 |
| Backbone-Backbone | 90 | 2.4 | 3 | 3.3 | 0.1 | 1 | 1.1 | 0.0 |
| Backbone-Sidechain | 212 | 5.6 | 18 | 8.5 | 0.5 | 1 | 0.5 | 0.0 |
| Sidechain-Sidechain | 95 | 2.5 | 3 | 3.2 | 0.1 | 0 | 0.0 | 0.0 |
| Long range ($i-j \geq 5$) | 1224 | 32.3 | 108 | 8.8 | 2.8 | 9 | 0.7 | 0.2 |
| Backbone-Backbone | 245 | 6.5 | 6 | 2.4 | 0.2 | 1 | 0.4 | 0.0 |
| Backbone-Sidechain | 604 | 15.9 | 67 | 11.1 | 1.8 | 6 | 1.0 | 0.2 |
| Sidechain-Sidechain | 375 | 9.9 | 35 | 9.3 | 0.9 | 2 | 0.5 | 0.1 |
| 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 | 74 | 2.0 | 1 | 1.4 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 3790 | 100.0 | 225 | 5.9 | 5.9 | 30 | 0.8 | 0.8 |
| Backbone-Backbone | 822 | 21.7 | 12 | 1.5 | 0.3 | 2 | 0.2 | 0.1 |
| Backbone-Sidechain | 2167 | 57.2 | 134 | 6.2 | 3.5 | 11 | 0.5 | 0.3 |
| Sidechain-Sidechain | 801 | 21.1 | 79 | 9.9 | 2.1 | 17 | 2.1 | 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 | 28 | 20 | 8 | 30 | 0 | 86 | 0.3 | 0.94 | 0.2 | 0.23 |
| 2 | 24 | 13 | 8 | 34 | 0 | 79 | 0.33 | 1.1 | 0.19 | 0.3 |
| 3 | 28 | 12 | 10 | 31 | 0 | 81 | 0.34 | 1.95 | 0.28 | 0.25 |
| 4 | 23 | 18 | 11 | 33 | 0 | 85 | 0.34 | 1.2 | 0.24 | 0.28 |
| 5 | 24 | 16 | 9 | 27 | 0 | 76 | 0.34 | 1.28 | 0.23 | 0.29 |
| 6 | 28 | 23 | 13 | 30 | 0 | 94 | 0.3 | 0.84 | 0.18 | 0.26 |
| 7 | 27 | 16 | 8 | 28 | 0 | 79 | 0.29 | 1.36 | 0.2 | 0.23 |
| 8 | 23 | 16 | 9 | 28 | 0 | 76 | 0.34 | 1.45 | 0.23 | 0.27 |
| 9 | 26 | 12 | 13 | 33 | 0 | 84 | 0.32 | 1.08 | 0.2 | 0.26 |
| 10 | 24 | 10 | 6 | 39 | 0 | 79 | 0.33 | 1.36 | 0.2 | 0.26 |

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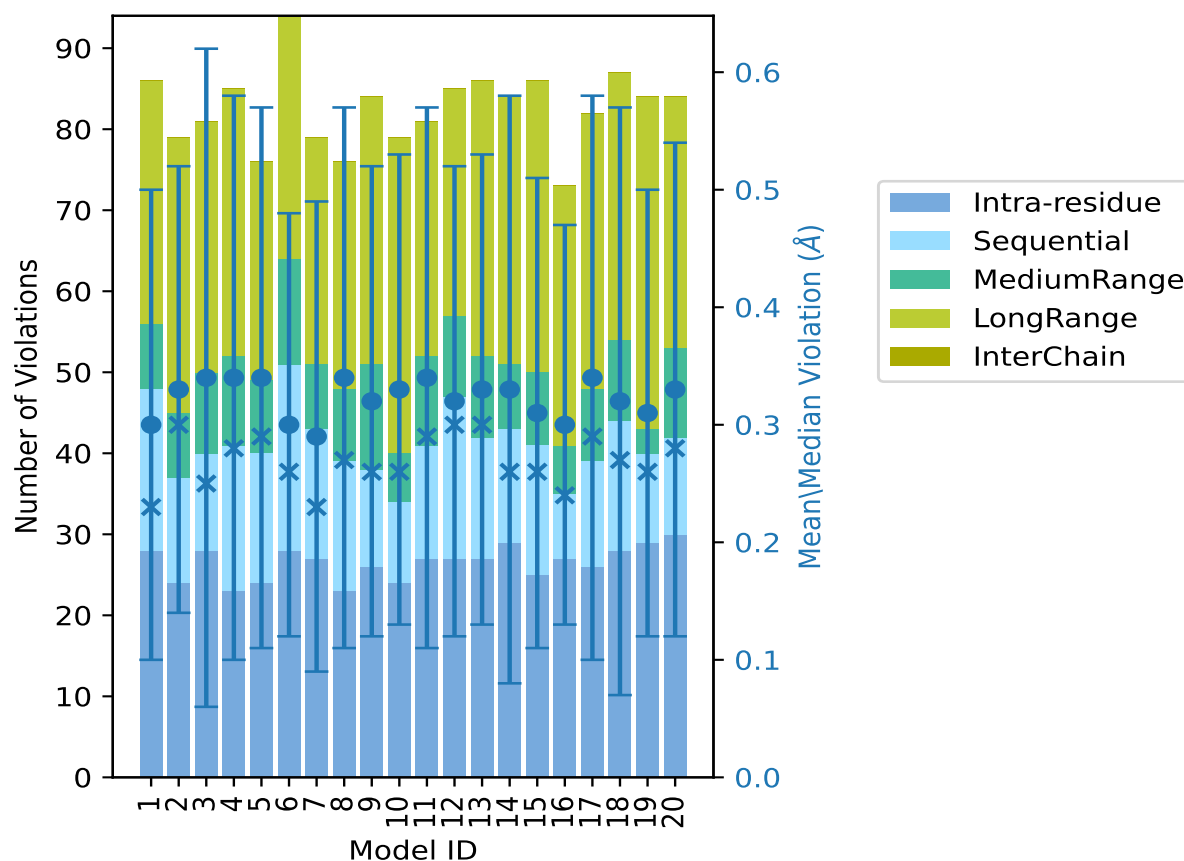
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 27 | 14 | 11 | 29 | 0 | 81 | 0.34 | 1.04 | 0.23 | 0.29 |
| 12 | 27 | 20 | 10 | 28 | 0 | 85 | 0.32 | 1.1 | 0.2 | 0.3 |
| 13 | 27 | 15 | 10 | 34 | 0 | 86 | 0.33 | 1.33 | 0.2 | 0.3 |
| 14 | 29 | 14 | 8 | 33 | 0 | 84 | 0.33 | 1.38 | 0.25 | 0.26 |
| 15 | 25 | 16 | 9 | 36 | 0 | 86 | 0.31 | 0.91 | 0.2 | 0.26 |
| 16 | 27 | 8 | 6 | 32 | 0 | 73 | 0.3 | 0.79 | 0.17 | 0.24 |
| 17 | 26 | 13 | 9 | 34 | 0 | 82 | 0.34 | 1.39 | 0.24 | 0.29 |
| 18 | 28 | 16 | 10 | 33 | 0 | 87 | 0.32 | 1.41 | 0.25 | 0.27 |
| 19 | 29 | 11 | 3 | 41 | 0 | 84 | 0.31 | 1.01 | 0.19 | 0.26 |
| 20 | 30 | 12 | 11 | 31 | 0 | 84 | 0.33 | 1.14 | 0.21 | 0.28 |

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

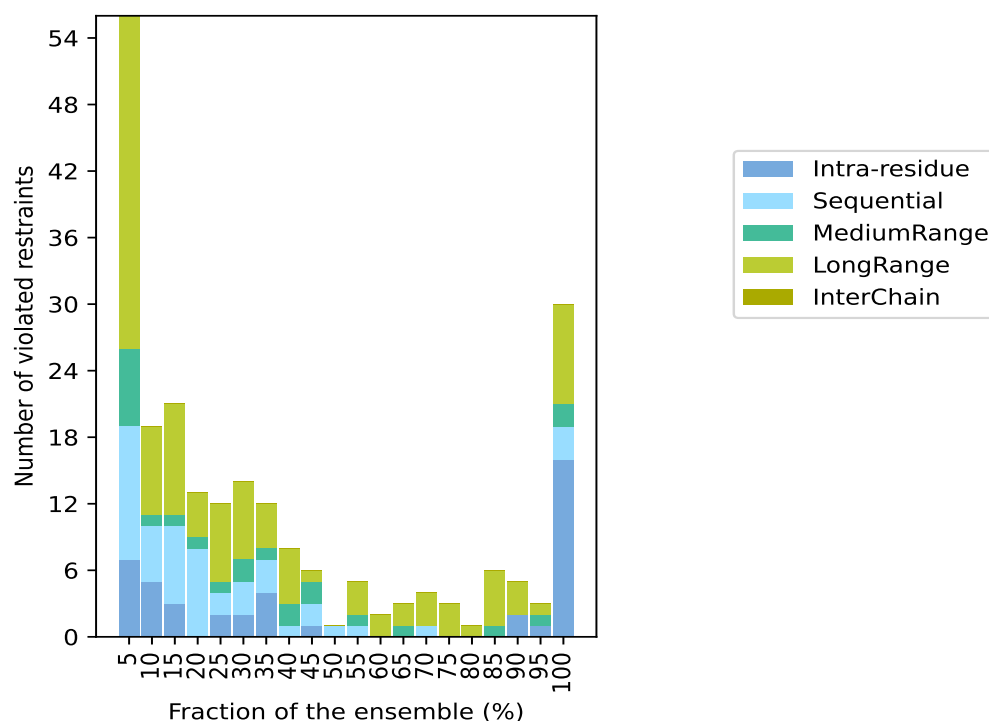
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3492(IR:1188, SQ:815, MR:373, LR:1116, IC:0) restraints are 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 | % |
| 7 | 12 | 7 | 30 | 0 | 56 | 1 | 5.0 |
| 5 | 5 | 1 | 8 | 0 | 19 | 2 | 10.0 |
| 3 | 7 | 1 | 10 | 0 | 21 | 3 | 15.0 |
| 0 | 8 | 1 | 4 | 0 | 13 | 4 | 20.0 |
| 2 | 2 | 1 | 7 | 0 | 12 | 5 | 25.0 |
| 2 | 3 | 2 | 7 | 0 | 14 | 6 | 30.0 |
| 4 | 3 | 1 | 4 | 0 | 12 | 7 | 35.0 |
| 0 | 1 | 2 | 5 | 0 | 8 | 8 | 40.0 |
| 1 | 2 | 2 | 1 | 0 | 6 | 9 | 45.0 |
| 0 | 1 | 0 | 0 | 0 | 1 | 10 | 50.0 |
| 0 | 1 | 1 | 3 | 0 | 5 | 11 | 55.0 |
| 0 | 0 | 0 | 2 | 0 | 2 | 12 | 60.0 |
| 0 | 0 | 1 | 2 | 0 | 3 | 13 | 65.0 |
| 0 | 1 | 0 | 3 | 0 | 4 | 14 | 70.0 |
| 0 | 0 | 0 | 3 | 0 | 3 | 15 | 75.0 |
| 0 | 0 | 0 | 1 | 0 | 1 | 16 | 80.0 |
| 0 | 0 | 1 | 5 | 0 | 6 | 17 | 85.0 |
| 2 | 0 | 0 | 3 | 0 | 5 | 18 | 90.0 |
| 1 | 0 | 1 | 1 | 0 | 3 | 19 | 95.0 |
| 16 | 3 | 2 | 9 | 0 | 30 | 20 | 100.0 |

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

⁵Inter-chain restraints, ⁶ Number of models with violations

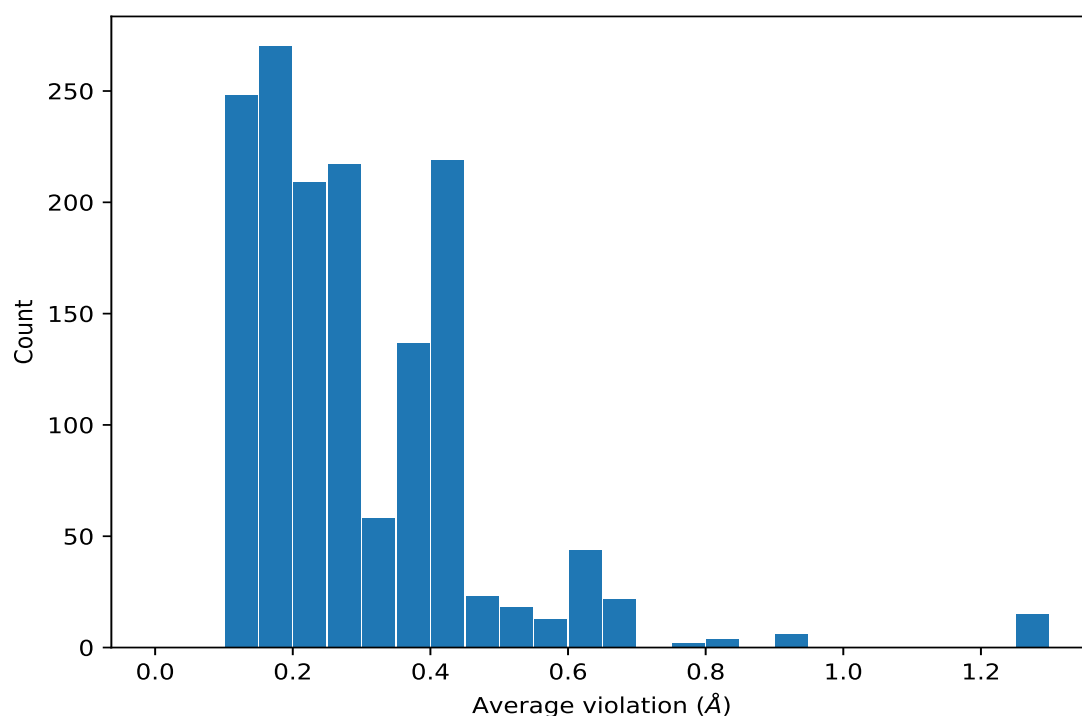
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 20 | 0.65 | 0.08 | 0.64 |
| (1,3133) | 1:42:A:PHE:H | 1:39:A:LYS:HA | 20 | 0.65 | 0.08 | 0.64 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG11 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG12 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG13 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG21 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG22 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG23 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 20 | 0.63 | 0.13 | 0.62 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 20 | 0.63 | 0.13 | 0.62 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG11 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG12 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG13 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG21 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG22 | 20 | 0.62 | 0.08 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG23 | 20 | 0.62 | 0.08 | 0.62 |
| (1,3672) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3672) | 1:41:A:THR:HG22 | 1:48:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3672) | 1:49:A:VAL:HG11 | 1:48:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3672) | 1:49:A:VAL:HG23 | 1:48:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3672) | 1:41:A:THR:HG21 | 1:48:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3672) | 1:49:A:VAL:HG12 | 1:48:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3672) | 1:49:A:VAL:HG13 | 1:48:A:THR:H | 20 | 0.61 | 0.16 | 0.61 |
| (1,3641) | 1:67:A:GLU:HB3 | 1:58:A:GLY:H | 20 | 0.6 | 0.23 | 0.62 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 20 | 0.6 | 0.23 | 0.62 |
| (1,3641) | 1:67:A:GLU:HG3 | 1:58:A:GLY:H | 20 | 0.6 | 0.23 | 0.62 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 20 | 0.57 | 0.16 | 0.5 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 20 | 0.57 | 0.16 | 0.5 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG2 | 20 | 0.57 | 0.16 | 0.5 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG3 | 20 | 0.57 | 0.16 | 0.5 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 20 | 0.51 | 0.13 | 0.51 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 20 | 0.51 | 0.13 | 0.51 |
| (1,3396) | 1:76:A:GLN:H | 1:56:A:ILE:HD11 | 20 | 0.51 | 0.13 | 0.51 |
| (1,3396) | 1:76:A:GLN:H | 1:56:A:ILE:HD12 | 20 | 0.51 | 0.13 | 0.51 |
| (1,3396) | 1:76:A:GLN:H | 1:56:A:ILE:HD13 | 20 | 0.51 | 0.13 | 0.51 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 | 0.01 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.42 | 0.02 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.42 | 0.02 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.4 | 0.02 | 0.41 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 | 0.02 | 0.37 |

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WORLDWIDE
PDB
PROTEIN DATA BANK

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 20 | 0.32 | 0.08 | 0.34 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.26 | 0.01 | 0.26 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 | 0.01 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 20 | 0.23 | 0.03 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 20 | 0.23 | 0.03 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 20 | 0.23 | 0.03 | 0.24 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 20 | 0.19 | 0.03 | 0.19 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 20 | 0.19 | 0.03 | 0.19 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 20 | 0.19 | 0.03 | 0.19 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.18 | 0.03 | 0.16 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.17 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.16 | 0.03 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.16 | 0.02 | 0.15 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 20 | 0.15 | 0.02 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 20 | 0.15 | 0.02 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 20 | 0.15 | 0.02 | 0.16 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 20 | 0.12 | 0.0 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 20 | 0.11 | 0.01 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 20 | 0.11 | 0.01 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 20 | 0.11 | 0.0 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 20 | 0.11 | 0.0 | 0.11 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG11 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG12 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG13 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG21 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG22 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG23 | 19 | 0.41 | 0.1 | 0.39 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 19 | 0.26 | 0.06 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 19 | 0.26 | 0.06 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HG2 | 19 | 0.26 | 0.06 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HG3 | 19 | 0.26 | 0.06 | 0.26 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 18 | 0.42 | 0.13 | 0.46 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 18 | 0.42 | 0.13 | 0.46 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 18 | 0.42 | 0.13 | 0.46 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 18 | 0.42 | 0.13 | 0.46 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 18 | 0.42 | 0.13 | 0.46 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.29 | 0.07 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.28 | 0.03 | 0.29 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.2 | 0.07 | 0.18 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 18 | 0.11 | 0.01 | 0.11 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:32:A:ALA:HA | 17 | 0.42 | 0.22 | 0.37 |
| (1,1405) | 1:29:A:ILE:HD13 | 1:32:A:ALA:HA | 17 | 0.42 | 0.22 | 0.37 |
| (1,1405) | 1:29:A:ILE:HD11 | 1:32:A:ALA:HA | 17 | 0.42 | 0.22 | 0.37 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:16:A:VAL:HA | 17 | 0.42 | 0.22 | 0.37 |
| (1,1405) | 1:29:A:ILE:HD13 | 1:16:A:VAL:HA | 17 | 0.42 | 0.22 | 0.37 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 17 | 0.37 | 0.11 | 0.4 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 17 | 0.37 | 0.11 | 0.4 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 17 | 0.37 | 0.11 | 0.4 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG2 | 17 | 0.37 | 0.11 | 0.4 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG3 | 17 | 0.37 | 0.11 | 0.4 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:29:A:ILE:HA | 17 | 0.35 | 0.17 | 0.35 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:31:A:THR:HB | 17 | 0.35 | 0.17 | 0.35 |
| (1,1331) | 1:12:A:VAL:HG11 | 1:29:A:ILE:HA | 17 | 0.35 | 0.17 | 0.35 |
| (1,1331) | 1:12:A:VAL:HG23 | 1:31:A:THR:HB | 17 | 0.35 | 0.17 | 0.35 |
| (1,1331) | 1:12:A:VAL:HG13 | 1:29:A:ILE:HA | 17 | 0.35 | 0.17 | 0.35 |
| (1,1331) | 1:12:A:VAL:HG21 | 1:31:A:THR:HB | 17 | 0.35 | 0.17 | 0.35 |
| (1,1331) | 1:12:A:VAL:HG23 | 1:29:A:ILE:HA | 17 | 0.35 | 0.17 | 0.35 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 17 | 0.35 | 0.14 | 0.34 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 17 | 0.35 | 0.14 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 17 | 0.3 | 0.09 | 0.29 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 17 | 0.16 | 0.04 | 0.16 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 17 | 0.16 | 0.04 | 0.16 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 16 | 0.43 | 0.13 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 16 | 0.43 | 0.13 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:93:A:PHE:HB2 | 16 | 0.43 | 0.13 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:93:A:PHE:HB3 | 16 | 0.43 | 0.13 | 0.42 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:50:A:GLU:HB2 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:50:A:GLU:HB3 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG22 | 1:38:A:VAL:HB | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:38:A:VAL:HB | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG11 | 1:38:A:VAL:HB | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG22 | 1:50:A:GLU:HG2 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG22 | 1:50:A:GLU:HG3 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG13 | 1:38:A:VAL:HB | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:38:A:VAL:HB | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG13 | 1:50:A:GLU:HG2 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG13 | 1:50:A:GLU:HG3 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG11 | 1:50:A:GLU:HB2 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG11 | 1:50:A:GLU:HB3 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:50:A:GLU:HB2 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:50:A:GLU:HB3 | 15 | 1.25 | 0.14 | 1.33 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 15 | 0.39 | 0.17 | 0.38 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 15 | 0.39 | 0.17 | 0.38 |
| (1,1947) | 1:40:A:VAL:HG12 | 1:79:A:VAL:HB | 15 | 0.39 | 0.17 | 0.38 |
| (1,1947) | 1:40:A:VAL:HG11 | 1:79:A:VAL:HB | 15 | 0.39 | 0.17 | 0.38 |
| (1,1947) | 1:91:A:VAL:HG11 | 1:30:A:LYS:HB2 | 15 | 0.39 | 0.17 | 0.38 |
| (1,1947) | 1:91:A:VAL:HG11 | 1:30:A:LYS:HB3 | 15 | 0.39 | 0.17 | 0.38 |
| (1,1947) | 1:91:A:VAL:HG12 | 1:30:A:LYS:HB2 | 15 | 0.39 | 0.17 | 0.38 |
| (1,1947) | 1:91:A:VAL:HG12 | 1:30:A:LYS:HB3 | 15 | 0.39 | 0.17 | 0.38 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 15 | 0.28 | 0.11 | 0.27 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 15 | 0.28 | 0.11 | 0.27 |
| (1,1819) | 1:28:A:LYS:HG2 | 1:29:A:ILE:HB | 14 | 0.7 | 0.29 | 0.76 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG2 | 14 | 0.7 | 0.29 | 0.76 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG3 | 14 | 0.7 | 0.29 | 0.76 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 14 | 0.7 | 0.29 | 0.76 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 14 | 0.3 | 0.07 | 0.3 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG11 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG11 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG12 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG12 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG13 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG13 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG21 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG21 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG22 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG22 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG23 | 14 | 0.3 | 0.07 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG23 | 14 | 0.3 | 0.07 | 0.3 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 14 | 0.26 | 0.09 | 0.26 |
| (1,1500) | 1:56:A:ILE:HD13 | 1:55:A:HIS:HA | 14 | 0.26 | 0.09 | 0.26 |
| (1,1500) | 1:56:A:ILE:HD12 | 1:55:A:HIS:HA | 14 | 0.26 | 0.09 | 0.26 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 14 | 0.21 | 0.06 | 0.2 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB2 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB3 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB2 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB3 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG21 | 1:88:A:TRP:HB2 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG21 | 1:88:A:TRP:HB3 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG22 | 1:30:A:LYS:HE2 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG22 | 1:30:A:LYS:HE3 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG23 | 1:30:A:LYS:HE2 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1622) | 1:90:A:THR:HG23 | 1:30:A:LYS:HE3 | 13 | 0.65 | 0.17 | 0.65 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:16:A:VAL:H | 13 | 0.53 | 0.23 | 0.67 |
| (1,1401) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 13 | 0.53 | 0.23 | 0.67 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:12:A:VAL:H | 13 | 0.53 | 0.23 | 0.67 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:16:A:VAL:H | 13 | 0.53 | 0.23 | 0.67 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 13 | 0.53 | 0.23 | 0.67 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 13 | 0.53 | 0.23 | 0.67 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 13 | 0.23 | 0.07 | 0.21 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 12 | 0.35 | 0.17 | 0.3 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 12 | 0.35 | 0.17 | 0.3 |
| (1,3585) | 1:84:A:THR:H | 1:36:A:VAL:HB | 12 | 0.35 | 0.17 | 0.3 |
| (1,3585) | 1:84:A:THR:H | 1:38:A:VAL:HB | 12 | 0.35 | 0.17 | 0.3 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 12 | 0.28 | 0.08 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 12 | 0.28 | 0.08 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 12 | 0.28 | 0.08 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:102:A:ARG:HG2 | 12 | 0.28 | 0.08 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:102:A:ARG:HG3 | 12 | 0.28 | 0.08 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3368) | 1:48:A:THR:HG22 | 1:41:A:THR:H | 11 | 0.42 | 0.2 | 0.44 |
| (1,3368) | 1:48:A:THR:HG23 | 1:41:A:THR:H | 11 | 0.42 | 0.2 | 0.44 |
| (1,3368) | 1:48:A:THR:HG21 | 1:41:A:THR:H | 11 | 0.42 | 0.2 | 0.44 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 11 | 0.33 | 0.11 | 0.33 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 11 | 0.33 | 0.11 | 0.33 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 11 | 0.29 | 0.06 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 11 | 0.29 | 0.06 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 11 | 0.29 | 0.06 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 11 | 0.29 | 0.06 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 11 | 0.29 | 0.06 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 11 | 0.29 | 0.06 | 0.29 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD11 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD12 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD13 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD21 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD22 | 11 | 0.21 | 0.15 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD23 | 11 | 0.21 | 0.15 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 11 | 0.17 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 11 | 0.17 | 0.03 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 11 | 0.17 | 0.03 | 0.16 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 10 | 0.36 | 0.17 | 0.32 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 10 | 0.36 | 0.17 | 0.32 |
| (1,3541) | 1:38:A:VAL:H | 1:37:A:LYS:HE2 | 10 | 0.36 | 0.17 | 0.32 |
| (1,3541) | 1:38:A:VAL:H | 1:37:A:LYS:HE3 | 10 | 0.36 | 0.17 | 0.32 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 9 | 0.46 | 0.24 | 0.43 |
| (1,3702) | 1:33:A:LYS:HE3 | 1:32:A:ALA:H | 9 | 0.46 | 0.24 | 0.43 |
| (1,3702) | 1:33:A:LYS:HE2 | 1:32:A:ALA:H | 9 | 0.46 | 0.24 | 0.43 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 9 | 0.39 | 0.06 | 0.42 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 9 | 0.39 | 0.06 | 0.42 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 9 | 0.17 | 0.02 | 0.17 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 9 | 0.13 | 0.02 | 0.13 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 9 | 0.13 | 0.02 | 0.13 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 9 | 0.13 | 0.03 | 0.12 |
| (1,3666) | 1:39:A:LYS:HG2 | 1:41:A:THR:H | 8 | 0.76 | 0.3 | 0.7 |
| (1,3666) | 1:39:A:LYS:HG3 | 1:41:A:THR:H | 8 | 0.76 | 0.3 | 0.7 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB2 | 8 | 0.47 | 0.14 | 0.5 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB3 | 8 | 0.47 | 0.14 | 0.5 |
| (1,1976) | 1:124:A:PRO:HD2 | 1:125:A:LEU:HB2 | 8 | 0.47 | 0.14 | 0.5 |
| (1,1976) | 1:124:A:PRO:HD2 | 1:125:A:LEU:HB3 | 8 | 0.47 | 0.14 | 0.5 |
| (1,1976) | 1:110:A:GLY:HA2 | 1:108:A:LEU:HB2 | 8 | 0.47 | 0.14 | 0.5 |
| (1,1976) | 1:110:A:GLY:HA2 | 1:108:A:LEU:HB3 | 8 | 0.47 | 0.14 | 0.5 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD21 | 8 | 0.4 | 0.14 | 0.42 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD22 | 8 | 0.4 | 0.14 | 0.42 |
| (1,3493) | 1:69:A:LYS:H | 1:42:A:PHE:HE1 | 8 | 0.4 | 0.14 | 0.42 |
| (1,3493) | 1:69:A:LYS:H | 1:42:A:PHE:HE2 | 8 | 0.4 | 0.14 | 0.42 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG2 | 8 | 0.38 | 0.14 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG3 | 8 | 0.38 | 0.14 | 0.38 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG2 | 8 | 0.38 | 0.14 | 0.38 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG3 | 8 | 0.38 | 0.14 | 0.38 |
| (1,1629) | 1:91:A:VAL:HG21 | 1:93:A:PHE:HA | 8 | 0.3 | 0.1 | 0.3 |
| (1,1629) | 1:91:A:VAL:HG22 | 1:99:A:LYS:HA | 8 | 0.3 | 0.1 | 0.3 |
| (1,1629) | 1:91:A:VAL:HG21 | 1:99:A:LYS:HA | 8 | 0.3 | 0.1 | 0.3 |
| (1,1629) | 1:91:A:VAL:HG22 | 1:27:A:ALA:HA | 8 | 0.3 | 0.1 | 0.3 |
| (1,1629) | 1:91:A:VAL:HG23 | 1:99:A:LYS:HA | 8 | 0.3 | 0.1 | 0.3 |
| (1,1629) | 1:91:A:VAL:HG22 | 1:93:A:PHE:HA | 8 | 0.3 | 0.1 | 0.3 |
| (1,1629) | 1:91:A:VAL:HG23 | 1:93:A:PHE:HA | 8 | 0.3 | 0.1 | 0.3 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG11 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG12 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG13 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG21 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG22 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG23 | 8 | 0.22 | 0.07 | 0.21 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 8 | 0.2 | 0.06 | 0.2 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 8 | 0.14 | 0.02 | 0.13 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 8 | 0.14 | 0.02 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 8 | 0.14 | 0.02 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 8 | 0.14 | 0.02 | 0.13 |
| (1,3714) | 1:115:A:ALA:HB1 | 1:114:A:PHE:H | 7 | 0.68 | 0.4 | 0.64 |
| (1,3714) | 1:115:A:ALA:HB3 | 1:114:A:PHE:H | 7 | 0.68 | 0.4 | 0.64 |
| (1,3714) | 1:112:A:ARG:HG2 | 1:114:A:PHE:H | 7 | 0.68 | 0.4 | 0.64 |
| (1,3680) | 1:19:A:LYS:HG3 | 1:24:A:PHE:H | 7 | 0.53 | 0.16 | 0.54 |
| (1,3680) | 1:38:A:VAL:HG23 | 1:53:A:ASP:H | 7 | 0.53 | 0.16 | 0.54 |
| (1,3680) | 1:38:A:VAL:HG22 | 1:53:A:ASP:H | 7 | 0.53 | 0.16 | 0.54 |
| (1,3680) | 1:38:A:VAL:HG12 | 1:53:A:ASP:H | 7 | 0.53 | 0.16 | 0.54 |
| (1,3680) | 1:38:A:VAL:HG13 | 1:53:A:ASP:H | 7 | 0.53 | 0.16 | 0.54 |
| (1,3662) | 1:112:A:ARG:HB3 | 1:113:A:HIS:H | 7 | 0.47 | 0.23 | 0.37 |
| (1,3662) | 1:120:A:LEU:HB3 | 1:121:A:ASP:H | 7 | 0.47 | 0.23 | 0.37 |
| (1,3662) | 1:112:A:ARG:HB2 | 1:113:A:HIS:H | 7 | 0.47 | 0.23 | 0.37 |
| (1,3611) | 1:13:A:GLY:HA3 | 1:12:A:VAL:H | 7 | 0.43 | 0.09 | 0.41 |
| (1,3611) | 1:105:A:SER:HB3 | 1:19:A:LYS:H | 7 | 0.43 | 0.09 | 0.41 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 7 | 0.4 | 0.18 | 0.44 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 7 | 0.4 | 0.18 | 0.44 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|----------------|---------------------|----------|---------------------|------------|
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG2 | 7 | 0.24 | 0.04 | 0.22 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG3 | 7 | 0.24 | 0.04 | 0.22 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HD2 | 7 | 0.24 | 0.04 | 0.22 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HD3 | 7 | 0.24 | 0.04 | 0.22 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.13 | 0.01 | 0.13 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 7 | 0.12 | 0.02 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 7 | 0.12 | 0.01 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 7 | 0.12 | 0.01 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 7 | 0.12 | 0.01 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 7 | 0.12 | 0.01 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 7 | 0.12 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 7 | 0.12 | 0.01 | 0.12 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 7 | 0.11 | 0.01 | 0.11 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 7 | 0.11 | 0.01 | 0.11 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 7 | 0.11 | 0.01 | 0.11 |
| (1,3664) | 1:101:A:LEU:HD12 | 1:106:A:LEU:H | 6 | 0.94 | 0.52 | 0.86 |
| (1,3664) | 1:120:A:LEU:HD23 | 1:122:A:GLN:H | 6 | 0.94 | 0.52 | 0.86 |
| (1,3664) | 1:120:A:LEU:HD13 | 1:122:A:GLN:H | 6 | 0.94 | 0.52 | 0.86 |
| (1,3664) | 1:101:A:LEU:HD21 | 1:106:A:LEU:H | 6 | 0.94 | 0.52 | 0.86 |
| (1,3664) | 1:101:A:LEU:HD11 | 1:106:A:LEU:H | 6 | 0.94 | 0.52 | 0.86 |
| (1,3664) | 1:101:A:LEU:HD22 | 1:106:A:LEU:H | 6 | 0.94 | 0.52 | 0.86 |
| (1,1644) | 1:101:A:LEU:HD13 | 1:105:A:SER:HA | 6 | 0.49 | 0.24 | 0.5 |
| (1,1644) | 1:101:A:LEU:HD21 | 1:99:A:LYS:HA | 6 | 0.49 | 0.24 | 0.5 |
| (1,1644) | 1:101:A:LEU:HD22 | 1:99:A:LYS:HA | 6 | 0.49 | 0.24 | 0.5 |
| (1,1644) | 1:101:A:LEU:HD11 | 1:99:A:LYS:HA | 6 | 0.49 | 0.24 | 0.5 |
| (1,1644) | 1:101:A:LEU:HD22 | 1:105:A:SER:HA | 6 | 0.49 | 0.24 | 0.5 |
| (1,3685) | 1:25:A:CYS:HB3 | 1:26:A:GLU:H | 6 | 0.42 | 0.09 | 0.4 |
| (1,3685) | 1:44:A:HIS:HB2 | 1:77:A:GLU:H | 6 | 0.42 | 0.09 | 0.4 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG21 | 6 | 0.38 | 0.07 | 0.39 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG22 | 6 | 0.38 | 0.07 | 0.39 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG23 | 6 | 0.38 | 0.07 | 0.39 |
| (1,3299) | 1:108:A:LEU:H | 1:10:A:LEU:HG | 6 | 0.32 | 0.14 | 0.27 |
| (1,3299) | 1:108:A:LEU:H | 1:109:A:LYS:HG2 | 6 | 0.32 | 0.14 | 0.27 |
| (1,3299) | 1:108:A:LEU:H | 1:109:A:LYS:HG3 | 6 | 0.32 | 0.14 | 0.27 |
| (1,1419) | 1:100:A:THR:HG23 | 1:89:A:TYR:H | 6 | 0.3 | 0.08 | 0.29 |
| (1,1419) | 1:100:A:THR:HG21 | 1:89:A:TYR:H | 6 | 0.3 | 0.08 | 0.29 |
| (1,1419) | 1:100:A:THR:HG22 | 1:89:A:TYR:H | 6 | 0.3 | 0.08 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 6 | 0.22 | 0.05 | 0.22 |
| (1,3214) | 1:57:A:LYS:H | 1:66:A:VAL:HB | 6 | 0.2 | 0.06 | 0.19 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD1 | 6 | 0.19 | 0.08 | 0.16 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD2 | 6 | 0.19 | 0.08 | 0.16 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG2 | 6 | 0.19 | 0.08 | 0.17 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG3 | 6 | 0.19 | 0.08 | 0.17 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.18 | 0.05 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.18 | 0.05 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 6 | 0.18 | 0.04 | 0.18 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB2 | 6 | 0.17 | 0.06 | 0.16 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB3 | 6 | 0.17 | 0.06 | 0.16 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HG | 6 | 0.17 | 0.06 | 0.16 |
| (1,3654) | 1:36:A:VAL:HB | 1:53:A:ASP:H | 6 | 0.13 | 0.02 | 0.12 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG21 | 5 | 0.33 | 0.05 | 0.33 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG22 | 5 | 0.33 | 0.05 | 0.33 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG23 | 5 | 0.33 | 0.05 | 0.33 |
| (1,3354) | 1:49:A:VAL:H | 1:39:A:LYS:HG2 | 5 | 0.33 | 0.05 | 0.33 |
| (1,3354) | 1:49:A:VAL:H | 1:39:A:LYS:HG3 | 5 | 0.33 | 0.05 | 0.33 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD11 | 5 | 0.32 | 0.12 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD12 | 5 | 0.32 | 0.12 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD13 | 5 | 0.32 | 0.12 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD21 | 5 | 0.32 | 0.12 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD22 | 5 | 0.32 | 0.12 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD23 | 5 | 0.32 | 0.12 | 0.4 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 5 | 0.27 | 0.06 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 5 | 0.27 | 0.06 | 0.27 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG2 | 5 | 0.26 | 0.08 | 0.23 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG3 | 5 | 0.26 | 0.08 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3671) | 1:65:A:ILE:HG12 | 1:66:A:VAL:H | 5 | 0.21 | 0.03 | 0.22 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG11 | 5 | 0.21 | 0.09 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG12 | 5 | 0.21 | 0.09 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG13 | 5 | 0.21 | 0.09 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG21 | 5 | 0.21 | 0.09 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG22 | 5 | 0.21 | 0.09 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG23 | 5 | 0.21 | 0.09 | 0.16 |
| (1,1402) | 1:29:A:ILE:HD11 | 1:17:A:SER:H | 5 | 0.19 | 0.13 | 0.13 |
| (1,1402) | 1:29:A:ILE:HD12 | 1:17:A:SER:H | 5 | 0.19 | 0.13 | 0.13 |
| (1,1402) | 1:29:A:ILE:HD13 | 1:17:A:SER:H | 5 | 0.19 | 0.13 | 0.13 |
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG2 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG2 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG3 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG3 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD2 | 1:91:A:VAL:HB | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG2 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG2 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG3 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG3 | 5 | 0.18 | 0.06 | 0.18 |
| (1,59) | 1:93:A:PHE:HD1 | 1:91:A:VAL:HB | 5 | 0.18 | 0.06 | 0.18 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.15 | 0.02 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.15 | 0.02 | 0.15 |
| (1,3116) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 5 | 0.12 | 0.03 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 5 | 0.12 | 0.03 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 5 | 0.12 | 0.03 | 0.11 |
| (1,1431) | 1:35:A:LEU:HG | 1:36:A:VAL:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,2481) | 1:80:A:ILE:HD11 | 1:80:A:ILE:H | 5 | 0.11 | 0.01 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD12 | 1:80:A:ILE:H | 5 | 0.11 | 0.01 | 0.1 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2481) | 1:80:A:ILE:HD13 | 1:80:A:ILE:H | 5 | 0.11 | 0.01 | 0.1 |
| (1,3652) | 1:98:A:GLU:HB3 | 1:99:A:LYS:H | 4 | 0.34 | 0.05 | 0.32 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD2 | 4 | 0.32 | 0.1 | 0.34 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD3 | 4 | 0.32 | 0.1 | 0.34 |
| (1,3640) | 1:81:A:ASN:HB2 | 1:41:A:THR:H | 4 | 0.29 | 0.22 | 0.18 |
| (1,1315) | 1:115:A:ALA:HA | 1:114:A:PHE:H | 4 | 0.28 | 0.15 | 0.23 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB1 | 4 | 0.22 | 0.09 | 0.21 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB2 | 4 | 0.22 | 0.09 | 0.21 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB3 | 4 | 0.22 | 0.09 | 0.21 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG2 | 4 | 0.22 | 0.07 | 0.2 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG3 | 4 | 0.22 | 0.07 | 0.2 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB2 | 4 | 0.22 | 0.06 | 0.22 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB3 | 4 | 0.22 | 0.06 | 0.22 |
| (1,770) | 1:60:A:LEU:HG | 1:59:A:PRO:HA | 4 | 0.19 | 0.01 | 0.2 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 4 | 0.17 | 0.07 | 0.14 |
| (1,3277) | 1:105:A:SER:H | 1:106:A:LEU:HG | 4 | 0.16 | 0.03 | 0.17 |
| (1,2447) | 1:99:A:LYS:HG2 | 1:98:A:GLU:H | 4 | 0.14 | 0.05 | 0.12 |
| (1,2447) | 1:99:A:LYS:HG3 | 1:98:A:GLU:H | 4 | 0.14 | 0.05 | 0.12 |
| (1,2618) | 1:9:A:TYR:HB2 | 1:10:A:LEU:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,2618) | 1:9:A:TYR:HB3 | 1:10:A:LEU:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,2464) | 1:10:A:LEU:HG | 1:11:A:THR:H | 4 | 0.11 | 0.01 | 0.11 |
| (1,1539) | 1:65:A:ILE:HD11 | 1:80:A:ILE:H | 3 | 0.67 | 0.39 | 0.51 |
| (1,1539) | 1:65:A:ILE:HD13 | 1:79:A:VAL:H | 3 | 0.67 | 0.39 | 0.51 |
| (1,1539) | 1:65:A:ILE:HD12 | 1:80:A:ILE:H | 3 | 0.67 | 0.39 | 0.51 |
| (1,1406) | 1:29:A:ILE:HD13 | 1:10:A:LEU:HG | 3 | 0.58 | 0.04 | 0.58 |
| (1,1406) | 1:29:A:ILE:HD12 | 1:10:A:LEU:HG | 3 | 0.58 | 0.04 | 0.58 |
| (1,3312) | 1:3:A:ALA:HB1 | 1:4:A:LEU:H | 3 | 0.5 | 0.14 | 0.53 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3312) | 1:3:A:ALA:HB2 | 1:4:A:LEU:H | 3 | 0.5 | 0.14 | 0.53 |
| (1,3599) | 1:76:A:GLN:HE21 | 1:76:A:GLN:HA | 3 | 0.39 | 0.37 | 0.14 |
| (1,3599) | 1:76:A:GLN:HE21 | 1:75:A:TYR:HA | 3 | 0.39 | 0.37 | 0.14 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG2 | 3 | 0.35 | 0.06 | 0.34 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG3 | 3 | 0.35 | 0.06 | 0.34 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD11 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD11 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD12 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD12 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD13 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD13 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD21 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD21 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD22 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD22 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD23 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD23 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:29:A:ILE:HG12 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:29:A:ILE:HG13 | 3 | 0.34 | 0.12 | 0.37 |
| (1,1376) | 1:32:A:ALA:HB1 | 1:89:A:TYR:HD1 | 3 | 0.33 | 0.33 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB1 | 1:89:A:TYR:HD2 | 3 | 0.33 | 0.33 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB2 | 1:89:A:TYR:HD1 | 3 | 0.33 | 0.33 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB2 | 1:89:A:TYR:HD2 | 3 | 0.33 | 0.33 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB3 | 1:89:A:TYR:HD1 | 3 | 0.33 | 0.33 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB3 | 1:89:A:TYR:HD2 | 3 | 0.33 | 0.33 | 0.1 |
| (1,1677) | 1:33:A:LYS:HB3 | 1:35:A:LEU:HG | 3 | 0.33 | 0.11 | 0.27 |
| (1,956) | 1:98:A:GLU:HG2 | 1:92:A:VAL:HB | 3 | 0.24 | 0.05 | 0.22 |
| (1,956) | 1:98:A:GLU:HG3 | 1:92:A:VAL:HB | 3 | 0.24 | 0.05 | 0.22 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG2 | 3 | 0.24 | 0.12 | 0.21 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG3 | 3 | 0.24 | 0.12 | 0.21 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD11 | 3 | 0.23 | 0.12 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD12 | 3 | 0.23 | 0.12 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD13 | 3 | 0.23 | 0.12 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD21 | 3 | 0.23 | 0.12 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD22 | 3 | 0.23 | 0.12 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD23 | 3 | 0.23 | 0.12 | 0.2 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG11 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG12 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG13 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG21 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG22 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG23 | 3 | 0.22 | 0.08 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG11 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG12 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG13 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG21 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG22 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG23 | 3 | 0.22 | 0.08 | 0.21 |
| (1,1382) | 1:27:A:ALA:HB3 | 1:26:A:GLU:HB2 | 3 | 0.21 | 0.1 | 0.18 |
| (1,1382) | 1:27:A:ALA:HB3 | 1:26:A:GLU:HB3 | 3 | 0.21 | 0.1 | 0.18 |
| (1,1382) | 1:27:A:ALA:HB2 | 1:16:A:VAL:HB | 3 | 0.21 | 0.1 | 0.18 |
| (1,1382) | 1:27:A:ALA:HB2 | 1:26:A:GLU:HB2 | 3 | 0.21 | 0.1 | 0.18 |
| (1,1382) | 1:27:A:ALA:HB2 | 1:26:A:GLU:HB3 | 3 | 0.21 | 0.1 | 0.18 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG2 | 3 | 0.2 | 0.01 | 0.21 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG3 | 3 | 0.2 | 0.01 | 0.21 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE2 | 3 | 0.19 | 0.0 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE3 | 3 | 0.19 | 0.0 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE2 | 3 | 0.19 | 0.0 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE3 | 3 | 0.19 | 0.0 | 0.19 |
| (1,3217) | 1:38:A:VAL:H | 1:38:A:VAL:HB | 3 | 0.17 | 0.04 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 3 | 0.16 | 0.03 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 3 | 0.16 | 0.03 | 0.15 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 3 | 0.16 | 0.04 | 0.17 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD2 | 3 | 0.15 | 0.02 | 0.15 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD3 | 3 | 0.15 | 0.02 | 0.15 |
| (1,3542) | 1:85:A:ASP:H | 1:83:A:LEU:HB2 | 3 | 0.15 | 0.07 | 0.1 |
| (1,3542) | 1:85:A:ASP:H | 1:83:A:LEU:HB3 | 3 | 0.15 | 0.07 | 0.1 |
| (1,3542) | 1:85:A:ASP:H | 1:37:A:LYS:HB2 | 3 | 0.15 | 0.07 | 0.1 |
| (1,3542) | 1:85:A:ASP:H | 1:37:A:LYS:HB3 | 3 | 0.15 | 0.07 | 0.1 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE2 | 3 | 0.13 | 0.01 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE3 | 3 | 0.13 | 0.01 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE2 | 3 | 0.13 | 0.01 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE3 | 3 | 0.13 | 0.01 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE2 | 3 | 0.13 | 0.01 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE3 | 3 | 0.13 | 0.01 | 0.12 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HE1 | 2 | 0.8 | 0.15 | 0.8 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HE2 | 2 | 0.8 | 0.15 | 0.8 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HD1 | 2 | 0.8 | 0.15 | 0.8 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HD2 | 2 | 0.8 | 0.15 | 0.8 |
| (1,1395) | 1:29:A:ILE:HA | 1:30:A:LYS:HG2 | 2 | 0.56 | 0.06 | 0.56 |
| (1,1395) | 1:29:A:ILE:HA | 1:30:A:LYS:HG3 | 2 | 0.56 | 0.06 | 0.56 |
| (1,1486) | 1:50:A:GLU:HG3 | 1:37:A:LYS:HA | 2 | 0.55 | 0.2 | 0.55 |
| (1,1486) | 1:50:A:GLU:HG2 | 1:38:A:VAL:HA | 2 | 0.55 | 0.2 | 0.55 |
| (1,3623) | 1:35:A:LEU:HA | 1:53:A:ASP:H | 2 | 0.38 | 0.11 | 0.38 |
| (1,3543) | 1:36:A:VAL:H | 1:85:A:ASP:HB2 | 2 | 0.31 | 0.13 | 0.31 |
| (1,3543) | 1:36:A:VAL:H | 1:85:A:ASP:HB3 | 2 | 0.31 | 0.13 | 0.31 |
| (1,3330) | 1:16:A:VAL:H | 1:109:A:LYS:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3330) | 1:16:A:VAL:H | 1:109:A:LYS:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3330) | 1:16:A:VAL:H | 1:28:A:LYS:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3330) | 1:16:A:VAL:H | 1:28:A:LYS:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3642) | 1:66:A:VAL:HB | 1:58:A:GLY:H | 2 | 0.22 | 0.04 | 0.22 |
| (1,3614) | 1:5:A:ASP:HA | 1:6:A:GLU:H | 2 | 0.21 | 0.01 | 0.21 |
| (1,3614) | 1:113:A:HIS:HA | 1:114:A:PHE:H | 2 | 0.21 | 0.01 | 0.21 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG11 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG11 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG12 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG12 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG13 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG13 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG21 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG21 | 2 | 0.2 | 0.1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG22 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG22 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG23 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG23 | 2 | 0.2 | 0.1 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,3258) | 1:109:A:LYS:H | 1:109:A:LYS:HB2 | 2 | 0.18 | 0.05 | 0.18 |
| (1,3258) | 1:109:A:LYS:H | 1:109:A:LYS:HB3 | 2 | 0.18 | 0.05 | 0.18 |
| (1,1341) | 1:16:A:VAL:HG13 | 1:89:A:TYR:HB2 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1341) | 1:16:A:VAL:HG13 | 1:89:A:TYR:HB3 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1341) | 1:16:A:VAL:HG22 | 1:89:A:TYR:HB2 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1341) | 1:16:A:VAL:HG22 | 1:89:A:TYR:HB3 | 2 | 0.15 | 0.0 | 0.15 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 2 | 0.14 | 0.02 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,1) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD1 | 2 | 0.13 | 0.01 | 0.13 |
| (1,1) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,1) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD1 | 2 | 0.13 | 0.01 | 0.13 |
| (1,1) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,2) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD1 | 2 | 0.13 | 0.01 | 0.13 |
| (1,2) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,2) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD1 | 2 | 0.13 | 0.01 | 0.13 |
| (1,2) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD2 | 2 | 0.13 | 0.01 | 0.13 |
| (1,3271) | 1:60:A:LEU:H | 1:60:A:LEU:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,3271) | 1:60:A:LEU:H | 1:60:A:LEU:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (2,73) | 1:109:A:LYS:H | 1:15:A:ASP:O | 2 | 0.11 | 0.01 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |

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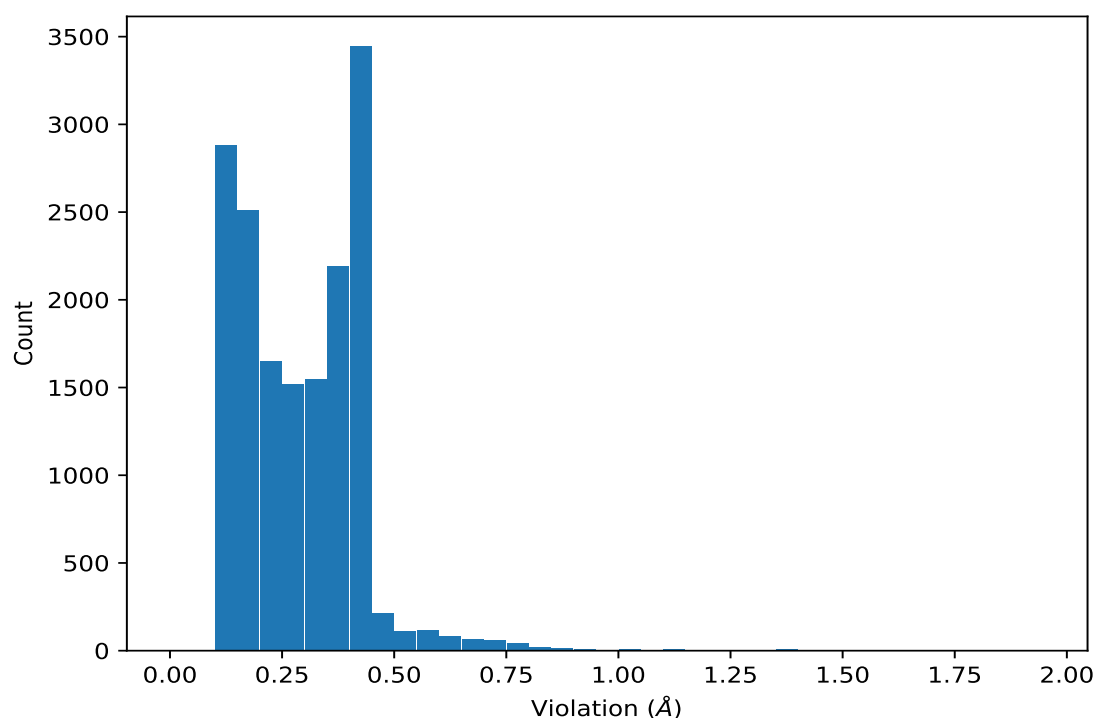
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 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) |
|----------|------------------|----------------|----------|---------------|
| (1,3664) | 1:101:A:LEU:HD12 | 1:106:A:LEU:H | 3 | 1.95 |
| (1,1490) | 1:51:A:VAL:HG22 | 1:50:A:GLU:HG2 | 8 | 1.45 |
| (1,1490) | 1:51:A:VAL:HG22 | 1:50:A:GLU:HG3 | 8 | 1.45 |
| (1,3714) | 1:115:A:ALA:HB3 | 1:114:A:PHE:H | 18 | 1.41 |
| (1,1490) | 1:51:A:VAL:HG11 | 1:50:A:GLU:HB2 | 17 | 1.39 |
| (1,1490) | 1:51:A:VAL:HG11 | 1:50:A:GLU:HB3 | 17 | 1.39 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:38:A:VAL:HB | 14 | 1.38 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:50:A:GLU:HB2 | 7 | 1.36 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:50:A:GLU:HB3 | 7 | 1.36 |
| (1,1490) | 1:51:A:VAL:HG13 | 1:38:A:VAL:HB | 10 | 1.36 |
| (1,1490) | 1:51:A:VAL:HG22 | 1:38:A:VAL:HB | 3 | 1.35 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:50:A:GLU:HB2 | 18 | 1.34 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:50:A:GLU:HB3 | 18 | 1.34 |
| (1,1490) | 1:51:A:VAL:HG13 | 1:50:A:GLU:HG2 | 13 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG13 | 1:50:A:GLU:HG3 | 13 | 1.33 |
| (1,1490) | 1:51:A:VAL:HG11 | 1:38:A:VAL:HB | 5 | 1.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3666) | 1:39:A:LYS:HG2 | 1:41:A:THR:H | 14 | 1.21 |
| (1,1539) | 1:65:A:ILE:HD13 | 1:79:A:VAL:H | 4 | 1.2 |
| (1,3641) | 1:67:A:GLU:HB3 | 1:58:A:GLY:H | 5 | 1.15 |
| (1,1490) | 1:51:A:VAL:HG11 | 1:38:A:VAL:HB | 20 | 1.14 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 18 | 1.12 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:38:A:VAL:HB | 4 | 1.11 |
| (1,3666) | 1:39:A:LYS:HG3 | 1:41:A:THR:H | 4 | 1.1 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:50:A:GLU:HB2 | 2 | 1.1 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:50:A:GLU:HB3 | 2 | 1.1 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:38:A:VAL:HB | 12 | 1.1 |
| (1,3664) | 1:120:A:LEU:HD23 | 1:122:A:GLN:H | 9 | 1.08 |
| (1,1490) | 1:51:A:VAL:HG12 | 1:38:A:VAL:HB | 11 | 1.04 |
| (1,3714) | 1:115:A:ALA:HB1 | 1:114:A:PHE:H | 4 | 1.03 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 17 | 1.03 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG2 | 3 | 1.03 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG3 | 3 | 1.03 |
| (1,3666) | 1:39:A:LYS:HG3 | 1:41:A:THR:H | 11 | 1.01 |
| (1,1490) | 1:51:A:VAL:HG21 | 1:38:A:VAL:HB | 19 | 1.01 |
| (1,1819) | 1:28:A:LYS:HG2 | 1:29:A:ILE:HB | 2 | 0.98 |
| (1,1405) | 1:29:A:ILE:HD13 | 1:16:A:VAL:HA | 14 | 0.98 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 8 | 0.95 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HD1 | 11 | 0.95 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HD2 | 11 | 0.95 |
| (1,3664) | 1:101:A:LEU:HD21 | 1:106:A:LEU:H | 18 | 0.94 |
| (1,1819) | 1:28:A:LYS:HG2 | 1:29:A:ILE:HB | 20 | 0.94 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB2 | 1 | 0.94 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB3 | 1 | 0.94 |
| (1,1644) | 1:101:A:LEU:HD22 | 1:99:A:LYS:HA | 12 | 0.92 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB2 | 17 | 0.92 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB3 | 17 | 0.92 |
| (1,3599) | 1:76:A:GLN:HE21 | 1:75:A:TYR:HA | 15 | 0.91 |
| (1,3672) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 1 | 0.9 |
| (1,3368) | 1:48:A:THR:HG22 | 1:41:A:THR:H | 14 | 0.89 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG2 | 9 | 0.89 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG3 | 9 | 0.89 |
| (1,3672) | 1:49:A:VAL:HG13 | 1:48:A:THR:H | 17 | 0.88 |
| (1,3509) | 1:87:A:SER:H | 1:89:A:TYR:HD1 | 11 | 0.86 |
| (1,3509) | 1:87:A:SER:H | 1:89:A:TYR:HD2 | 11 | 0.86 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG2 | 3 | 0.85 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG3 | 3 | 0.85 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 19 | 0.85 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 19 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 19 | 0.85 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 19 | 0.85 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 19 | 0.85 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 19 | 0.85 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 11 | 0.84 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG2 | 15 | 0.84 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG3 | 15 | 0.84 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 6 | 0.84 |
| (1,3680) | 1:38:A:VAL:HG22 | 1:53:A:ASP:H | 12 | 0.83 |
| (1,3662) | 1:112:A:ARG:HB3 | 1:113:A:HIS:H | 8 | 0.83 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 14 | 0.83 |
| (1,3585) | 1:84:A:THR:H | 1:36:A:VAL:HB | 4 | 0.83 |
| (1,3641) | 1:67:A:GLU:HB3 | 1:58:A:GLY:H | 1 | 0.81 |
| (1,3666) | 1:39:A:LYS:HG2 | 1:41:A:THR:H | 15 | 0.8 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 10 | 0.8 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 11 | 0.8 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 11 | 0.8 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 5 | 0.8 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 5 | 0.8 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 5 | 0.8 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 5 | 0.8 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 5 | 0.8 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 5 | 0.8 |
| (1,1622) | 1:90:A:THR:HG21 | 1:88:A:TRP:HB2 | 10 | 0.8 |
| (1,1622) | 1:90:A:THR:HG21 | 1:88:A:TRP:HB3 | 10 | 0.8 |
| (1,3672) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 16 | 0.79 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 1 | 0.79 |
| (1,1376) | 1:32:A:ALA:HB3 | 1:89:A:TYR:HD1 | 14 | 0.79 |
| (1,1376) | 1:32:A:ALA:HB3 | 1:89:A:TYR:HD2 | 14 | 0.79 |
| (1,3664) | 1:101:A:LEU:HD11 | 1:106:A:LEU:H | 19 | 0.78 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG2 | 20 | 0.78 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG3 | 20 | 0.78 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG11 | 1 | 0.78 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG12 | 1 | 0.78 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG13 | 1 | 0.78 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG21 | 1 | 0.78 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG22 | 1 | 0.78 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG23 | 1 | 0.78 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 18 | 0.78 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 18 | 0.78 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 18 | 0.78 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 18 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 18 | 0.78 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 18 | 0.78 |
| (1,3662) | 1:112:A:ARG:HB3 | 1:113:A:HIS:H | 6 | 0.77 |
| (1,3641) | 1:67:A:GLU:HG3 | 1:58:A:GLY:H | 20 | 0.77 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 2 | 0.77 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 4 | 0.77 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 11 | 0.77 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 5 | 0.76 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 5 | 0.76 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 7 | 0.76 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 7 | 0.76 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 7 | 0.76 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 7 | 0.76 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 7 | 0.76 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 7 | 0.76 |
| (1,1486) | 1:50:A:GLU:HG2 | 1:38:A:VAL:HA | 6 | 0.76 |
| (1,1456) | 1:92:A:VAL:HB | 1:93:A:PHE:HB2 | 11 | 0.76 |
| (1,1456) | 1:92:A:VAL:HB | 1:93:A:PHE:HB3 | 11 | 0.76 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 17 | 0.75 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG11 | 9 | 0.75 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG12 | 9 | 0.75 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG13 | 9 | 0.75 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG21 | 9 | 0.75 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG22 | 9 | 0.75 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG23 | 9 | 0.75 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 13 | 0.74 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 1 | 0.74 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 1 | 0.74 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 1 | 0.74 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 1 | 0.74 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 1 | 0.74 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 1 | 0.74 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 1 | 0.74 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 1 | 0.74 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG11 | 20 | 0.74 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG12 | 20 | 0.74 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG13 | 20 | 0.74 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG21 | 20 | 0.74 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG22 | 20 | 0.74 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG23 | 20 | 0.74 |
| (1,1622) | 1:90:A:THR:HG21 | 1:88:A:TRP:HB2 | 9 | 0.74 |
| (1,1622) | 1:90:A:THR:HG21 | 1:88:A:TRP:HB3 | 9 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1401) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 5 | 0.74 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 16 | 0.74 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 4 | 0.73 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 4 | 0.73 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 13 | 0.73 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 13 | 0.73 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG2 | 12 | 0.73 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG3 | 12 | 0.73 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 17 | 0.73 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG11 | 17 | 0.73 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG12 | 17 | 0.73 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG13 | 17 | 0.73 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG21 | 17 | 0.73 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG22 | 17 | 0.73 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG23 | 17 | 0.73 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 7 | 0.72 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 18 | 0.72 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 18 | 0.72 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 18 | 0.72 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 18 | 0.72 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 18 | 0.72 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 18 | 0.72 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:16:A:VAL:HA | 10 | 0.72 |
| (1,1947) | 1:40:A:VAL:HG11 | 1:79:A:VAL:HB | 6 | 0.71 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 8 | 0.71 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 8 | 0.71 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 8 | 0.71 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 8 | 0.71 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 8 | 0.71 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 8 | 0.71 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB2 | 3 | 0.71 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB3 | 3 | 0.71 |
| (1,1622) | 1:90:A:THR:HG23 | 1:30:A:LYS:HE2 | 16 | 0.71 |
| (1,1622) | 1:90:A:THR:HG23 | 1:30:A:LYS:HE3 | 16 | 0.71 |
| (1,3714) | 1:112:A:ARG:HG2 | 1:114:A:PHE:H | 13 | 0.7 |
| (1,3672) | 1:49:A:VAL:HG12 | 1:48:A:THR:H | 14 | 0.7 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 15 | 0.7 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 9 | 0.7 |
| (1,1691) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 6 | 0.7 |
| (1,1691) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 6 | 0.7 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 15 | 0.7 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 9 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 9 | 0.69 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 9 | 0.69 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 9 | 0.69 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 9 | 0.69 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 9 | 0.69 |
| (1,3672) | 1:41:A:THR:HG21 | 1:48:A:THR:H | 8 | 0.68 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 12 | 0.68 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG11 | 8 | 0.68 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG12 | 8 | 0.68 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG13 | 8 | 0.68 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG21 | 8 | 0.68 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG22 | 8 | 0.68 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG23 | 8 | 0.68 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:32:A:ALA:HA | 15 | 0.68 |
| (1,1401) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 12 | 0.68 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 19 | 0.68 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 13 | 0.67 |
| (1,3640) | 1:81:A:ASN:HB2 | 1:41:A:THR:H | 13 | 0.67 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 16 | 0.67 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 16 | 0.67 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 12 | 0.67 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 17 | 0.67 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 17 | 0.67 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 17 | 0.67 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 17 | 0.67 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 17 | 0.67 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 17 | 0.67 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:16:A:VAL:H | 17 | 0.67 |
| (1,3672) | 1:49:A:VAL:HG23 | 1:48:A:THR:H | 15 | 0.66 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 20 | 0.66 |
| (1,3663) | 1:30:A:LYS:HG3 | 1:92:A:VAL:H | 20 | 0.66 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 8 | 0.66 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 8 | 0.66 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 16 | 0.66 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 20 | 0.66 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 20 | 0.66 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 20 | 0.66 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 20 | 0.66 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 20 | 0.66 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 20 | 0.66 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 7 | 0.66 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 7 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 7 | 0.66 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 7 | 0.66 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 7 | 0.66 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 7 | 0.66 |
| (1,1491) | 1:51:A:VAL:HG21 | 1:40:A:VAL:HG11 | 2 | 0.66 |
| (1,1491) | 1:51:A:VAL:HG21 | 1:40:A:VAL:HG12 | 2 | 0.66 |
| (1,1491) | 1:51:A:VAL:HG21 | 1:40:A:VAL:HG13 | 2 | 0.66 |
| (1,1491) | 1:51:A:VAL:HG21 | 1:40:A:VAL:HG21 | 2 | 0.66 |
| (1,1491) | 1:51:A:VAL:HG21 | 1:40:A:VAL:HG22 | 2 | 0.66 |
| (1,1491) | 1:51:A:VAL:HG21 | 1:40:A:VAL:HG23 | 2 | 0.66 |
| (1,3672) | 1:49:A:VAL:HG11 | 1:48:A:THR:H | 18 | 0.65 |
| (1,3664) | 1:120:A:LEU:HD13 | 1:122:A:GLN:H | 12 | 0.65 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 2 | 0.65 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 2 | 0.65 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 2 | 0.65 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 2 | 0.65 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 2 | 0.65 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 2 | 0.65 |
| (1,3312) | 1:3:A:ALA:HB1 | 1:4:A:LEU:H | 17 | 0.65 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 6 | 0.65 |
| (1,1976) | 1:110:A:GLY:HA2 | 1:108:A:LEU:HB2 | 8 | 0.65 |
| (1,1976) | 1:110:A:GLY:HA2 | 1:108:A:LEU:HB3 | 8 | 0.65 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB2 | 4 | 0.65 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB3 | 4 | 0.65 |
| (1,3714) | 1:115:A:ALA:HB3 | 1:114:A:PHE:H | 7 | 0.64 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 5 | 0.64 |
| (1,3133) | 1:42:A:PHE:H | 1:39:A:LYS:HA | 15 | 0.64 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG11 | 14 | 0.64 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG12 | 14 | 0.64 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG13 | 14 | 0.64 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG21 | 14 | 0.64 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG22 | 14 | 0.64 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG23 | 14 | 0.64 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 3 | 0.64 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 3 | 0.64 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 3 | 0.64 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 3 | 0.64 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 3 | 0.64 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 3 | 0.64 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HE1 | 9 | 0.64 |
| (1,1558) | 1:97:A:ASP:HB3 | 1:20:A:TYR:HE2 | 9 | 0.64 |
| (1,1331) | 1:12:A:VAL:HG13 | 1:29:A:ILE:HA | 9 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 15 | 0.63 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 15 | 0.63 |
| (1,3396) | 1:76:A:GLN:H | 1:56:A:ILE:HD11 | 17 | 0.63 |
| (1,3396) | 1:76:A:GLN:H | 1:56:A:ILE:HD12 | 17 | 0.63 |
| (1,3396) | 1:76:A:GLN:H | 1:56:A:ILE:HD13 | 17 | 0.63 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 13 | 0.63 |
| (1,3133) | 1:42:A:PHE:H | 1:39:A:LYS:HA | 20 | 0.63 |
| (1,1947) | 1:91:A:VAL:HG11 | 1:30:A:LYS:HB2 | 8 | 0.63 |
| (1,1947) | 1:91:A:VAL:HG11 | 1:30:A:LYS:HB3 | 8 | 0.63 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 12 | 0.63 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 12 | 0.63 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 12 | 0.63 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 12 | 0.63 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 12 | 0.63 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 12 | 0.63 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:29:A:ILE:HA | 2 | 0.63 |
| (1,3672) | 1:49:A:VAL:HG11 | 1:48:A:THR:H | 5 | 0.62 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 8 | 0.62 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 10 | 0.62 |
| (1,1695) | 1:108:A:LEU:HD13 | 1:9:A:TYR:HB2 | 17 | 0.62 |
| (1,1695) | 1:108:A:LEU:HD13 | 1:9:A:TYR:HB2 | 17 | 0.62 |
| (1,1695) | 1:108:A:LEU:HD13 | 1:9:A:TYR:HB3 | 17 | 0.62 |
| (1,1695) | 1:108:A:LEU:HD13 | 1:9:A:TYR:HB3 | 17 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG11 | 5 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG12 | 5 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG13 | 5 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG21 | 5 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG22 | 5 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG23 | 5 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG11 | 14 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG12 | 14 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG13 | 14 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG21 | 14 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG22 | 14 | 0.62 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG23 | 14 | 0.62 |
| (1,1406) | 1:29:A:ILE:HD13 | 1:10:A:LEU:HG | 19 | 0.62 |
| (1,1395) | 1:29:A:ILE:HA | 1:30:A:LYS:HG2 | 20 | 0.62 |
| (1,1395) | 1:29:A:ILE:HA | 1:30:A:LYS:HG3 | 20 | 0.62 |
| (1,3680) | 1:38:A:VAL:HG22 | 1:53:A:ASP:H | 19 | 0.61 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 7 | 0.61 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 9 | 0.61 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 9 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 18 | 0.61 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 16 | 0.61 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 16 | 0.61 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 16 | 0.61 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 16 | 0.61 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 16 | 0.61 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 16 | 0.61 |
| (1,3685) | 1:44:A:HIS:HB2 | 1:77:A:GLU:H | 9 | 0.6 |
| (1,3672) | 1:41:A:THR:HG21 | 1:48:A:THR:H | 11 | 0.6 |
| (1,3666) | 1:39:A:LYS:HG2 | 1:41:A:THR:H | 5 | 0.6 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 3 | 0.6 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 1 | 0.6 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 1 | 0.6 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 1 | 0.6 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 20 | 0.6 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 20 | 0.6 |
| (1,1947) | 1:40:A:VAL:HG12 | 1:79:A:VAL:HB | 9 | 0.6 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 4 | 0.6 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 4 | 0.6 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 4 | 0.6 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 4 | 0.6 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 4 | 0.6 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 4 | 0.6 |
| (1,3680) | 1:38:A:VAL:HG23 | 1:53:A:ASP:H | 11 | 0.59 |
| (1,3672) | 1:41:A:THR:HG22 | 1:48:A:THR:H | 12 | 0.59 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 15 | 0.59 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 15 | 0.59 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 15 | 0.59 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 14 | 0.59 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 14 | 0.59 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 10 | 0.59 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 10 | 0.59 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 19 | 0.59 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 15 | 0.59 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 15 | 0.59 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 15 | 0.59 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 15 | 0.59 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 15 | 0.59 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 15 | 0.59 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG11 | 5 | 0.58 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG12 | 5 | 0.58 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG13 | 5 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG21 | 5 | 0.58 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG22 | 5 | 0.58 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG23 | 5 | 0.58 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 14 | 0.58 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 4 | 0.58 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 10 | 0.58 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 10 | 0.58 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 10 | 0.58 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 10 | 0.58 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 10 | 0.58 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 10 | 0.58 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB2 | 14 | 0.58 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB3 | 14 | 0.58 |
| (1,1406) | 1:29:A:ILE:HD12 | 1:10:A:LEU:HG | 5 | 0.58 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 2 | 0.57 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 5 | 0.57 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 5 | 0.57 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 20 | 0.57 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 20 | 0.57 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG2 | 5 | 0.57 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG3 | 5 | 0.57 |
| (1,3133) | 1:42:A:PHE:H | 1:39:A:LYS:HA | 3 | 0.57 |
| (1,1976) | 1:124:A:PRO:HD2 | 1:125:A:LEU:HB2 | 3 | 0.57 |
| (1,1976) | 1:124:A:PRO:HD2 | 1:125:A:LEU:HB3 | 3 | 0.57 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 19 | 0.57 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 19 | 0.57 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 3 | 0.57 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 3 | 0.57 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 3 | 0.57 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 3 | 0.57 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 3 | 0.57 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 3 | 0.57 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG11 | 15 | 0.57 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG12 | 15 | 0.57 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG13 | 15 | 0.57 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG21 | 15 | 0.57 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG22 | 15 | 0.57 |
| (1,1692) | 1:41:A:THR:HG23 | 1:79:A:VAL:HG23 | 15 | 0.57 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 19 | 0.57 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 19 | 0.57 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 19 | 0.57 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 19 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 19 | 0.57 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 19 | 0.57 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB2 | 6 | 0.57 |
| (1,1622) | 1:90:A:THR:HG22 | 1:88:A:TRP:HB3 | 6 | 0.57 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 17 | 0.57 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 17 | 0.57 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:16:A:VAL:H | 2 | 0.57 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 4 | 0.56 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 19 | 0.56 |
| (1,3662) | 1:112:A:ARG:HB3 | 1:113:A:HIS:H | 13 | 0.56 |
| (1,3611) | 1:13:A:GLY:HA3 | 1:12:A:VAL:H | 4 | 0.56 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 4 | 0.56 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 4 | 0.56 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 10 | 0.56 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 10 | 0.56 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 18 | 0.56 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 18 | 0.56 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD21 | 6 | 0.56 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD22 | 6 | 0.56 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG11 | 9 | 0.56 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG12 | 9 | 0.56 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG13 | 9 | 0.56 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG21 | 9 | 0.56 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG22 | 9 | 0.56 |
| (1,3389) | 1:64:A:ALA:H | 1:62:A:VAL:HG23 | 9 | 0.56 |
| (1,3368) | 1:48:A:THR:HG21 | 1:41:A:THR:H | 10 | 0.56 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG2 | 13 | 0.56 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG3 | 13 | 0.56 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 4 | 0.56 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 4 | 0.56 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 4 | 0.56 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 4 | 0.56 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 4 | 0.56 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 4 | 0.56 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB2 | 18 | 0.56 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB3 | 18 | 0.56 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 19 | 0.56 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 19 | 0.56 |
| (1,1405) | 1:29:A:ILE:HD11 | 1:32:A:ALA:HA | 17 | 0.56 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 2 | 0.55 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 7 | 0.55 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD21 | 8 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD22 | 8 | 0.55 |
| (1,3299) | 1:108:A:LEU:H | 1:109:A:LYS:HG2 | 11 | 0.55 |
| (1,3299) | 1:108:A:LEU:H | 1:109:A:LYS:HG3 | 11 | 0.55 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 16 | 0.55 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 16 | 0.55 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 16 | 0.55 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 16 | 0.55 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 16 | 0.55 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 16 | 0.55 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 13 | 0.55 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 13 | 0.55 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 13 | 0.55 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 13 | 0.55 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 13 | 0.55 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 13 | 0.55 |
| (1,1331) | 1:12:A:VAL:HG21 | 1:31:A:THR:HB | 11 | 0.55 |
| (1,3680) | 1:38:A:VAL:HG23 | 1:53:A:ASP:H | 9 | 0.54 |
| (1,3666) | 1:39:A:LYS:HG2 | 1:41:A:THR:H | 12 | 0.54 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 11 | 0.54 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 11 | 0.54 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 11 | 0.54 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 6 | 0.54 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 6 | 0.54 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 6 | 0.54 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 6 | 0.54 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 6 | 0.54 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 6 | 0.54 |
| (1,1644) | 1:101:A:LEU:HD13 | 1:105:A:SER:HA | 2 | 0.54 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 3 | 0.53 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 3 | 0.53 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 6 | 0.53 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 6 | 0.53 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 9 | 0.53 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 9 | 0.53 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 15 | 0.53 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 15 | 0.53 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 15 | 0.53 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 15 | 0.53 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 15 | 0.53 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 15 | 0.53 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG2 | 8 | 0.53 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG3 | 8 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3312) | 1:3:A:ALA:HB2 | 1:4:A:LEU:H | 19 | 0.53 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 1 | 0.53 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 1 | 0.53 |
| (1,3133) | 1:42:A:PHE:H | 1:39:A:LYS:HA | 8 | 0.53 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB2 | 2 | 0.53 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB3 | 2 | 0.53 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 12 | 0.53 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 12 | 0.53 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 12 | 0.53 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 12 | 0.53 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 12 | 0.53 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 12 | 0.53 |
| (1,1644) | 1:101:A:LEU:HD13 | 1:105:A:SER:HA | 13 | 0.53 |
| (1,1406) | 1:29:A:ILE:HD13 | 1:10:A:LEU:HG | 15 | 0.53 |
| (1,1315) | 1:115:A:ALA:HA | 1:114:A:PHE:H | 3 | 0.53 |
| (1,3714) | 1:115:A:ALA:HB3 | 1:114:A:PHE:H | 11 | 0.52 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 3 | 0.52 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 16 | 0.52 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 16 | 0.52 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD21 | 15 | 0.52 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD22 | 15 | 0.52 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG2 | 3 | 0.52 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG3 | 3 | 0.52 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 14 | 0.52 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 14 | 0.52 |
| (1,1754) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HA | 2 | 0.52 |
| (1,1754) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HA | 8 | 0.52 |
| (1,1754) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HA | 19 | 0.52 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB2 | 5 | 0.52 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB3 | 5 | 0.52 |
| (1,1331) | 1:12:A:VAL:HG13 | 1:29:A:ILE:HA | 19 | 0.52 |
| (1,3611) | 1:13:A:GLY:HA3 | 1:12:A:VAL:H | 3 | 0.51 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 10 | 0.51 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 10 | 0.51 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 10 | 0.51 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 10 | 0.51 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 10 | 0.51 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 10 | 0.51 |
| (1,3368) | 1:48:A:THR:HG23 | 1:41:A:THR:H | 7 | 0.51 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 10 | 0.51 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 10 | 0.51 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 2 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 2 | 0.51 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 6 | 0.51 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 6 | 0.51 |
| (1,3133) | 1:42:A:PHE:H | 1:79:A:VAL:HA | 11 | 0.51 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB2 | 13 | 0.51 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB3 | 13 | 0.51 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 15 | 0.51 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 15 | 0.51 |
| (1,1754) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HA | 7 | 0.51 |
| (1,1754) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HA | 9 | 0.51 |
| (1,1754) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HA | 20 | 0.51 |
| (1,1539) | 1:65:A:ILE:HD11 | 1:80:A:ILE:H | 1 | 0.51 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 12 | 0.5 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 3 | 0.5 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 3 | 0.5 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 20 | 0.5 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 20 | 0.5 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 20 | 0.5 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 18 | 0.5 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 18 | 0.5 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 18 | 0.5 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 18 | 0.5 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 18 | 0.5 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 18 | 0.5 |
| (1,3368) | 1:48:A:THR:HG23 | 1:41:A:THR:H | 4 | 0.5 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 5 | 0.5 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 5 | 0.5 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 17 | 0.5 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 17 | 0.5 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 19 | 0.5 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 19 | 0.5 |
| (1,1707) | 1:120:A:LEU:HD23 | 1:120:A:LEU:HA | 16 | 0.5 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG11 | 11 | 0.5 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG12 | 11 | 0.5 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG13 | 11 | 0.5 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG21 | 11 | 0.5 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG22 | 11 | 0.5 |
| (1,1692) | 1:41:A:THR:HG22 | 1:79:A:VAL:HG23 | 11 | 0.5 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:16:A:VAL:H | 7 | 0.5 |
| (1,1395) | 1:29:A:ILE:HA | 1:30:A:LYS:HG2 | 3 | 0.5 |
| (1,1395) | 1:29:A:ILE:HA | 1:30:A:LYS:HG3 | 3 | 0.5 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 8 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3623) | 1:35:A:LEU:HA | 1:53:A:ASP:H | 1 | 0.49 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 13 | 0.49 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 13 | 0.49 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 18 | 0.49 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 18 | 0.49 |
| (1,1976) | 1:124:A:PRO:HD2 | 1:125:A:LEU:HB2 | 18 | 0.49 |
| (1,1976) | 1:124:A:PRO:HD2 | 1:125:A:LEU:HB3 | 18 | 0.49 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB2 | 20 | 0.49 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB3 | 20 | 0.49 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 10 | 0.49 |
| (1,1754) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HA | 16 | 0.49 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 10 | 0.49 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 10 | 0.49 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 10 | 0.49 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 10 | 0.49 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 10 | 0.49 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 10 | 0.49 |
| (1,1405) | 1:29:A:ILE:HD13 | 1:32:A:ALA:HA | 18 | 0.49 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 20 | 0.48 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 20 | 0.48 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 5 | 0.48 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 5 | 0.48 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG21 | 13 | 0.48 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG22 | 13 | 0.48 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG23 | 13 | 0.48 |
| (1,1754) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HA | 3 | 0.48 |
| (1,1754) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HA | 5 | 0.48 |
| (1,1754) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HA | 15 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 11 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 11 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 11 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 11 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 11 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 11 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG11 | 13 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG12 | 13 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG13 | 13 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG21 | 13 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG22 | 13 | 0.48 |
| (1,1735) | 1:93:A:PHE:HD2 | 1:92:A:VAL:HG23 | 13 | 0.48 |
| (1,1677) | 1:33:A:LYS:HB3 | 1:35:A:LEU:HG | 4 | 0.48 |
| (1,3611) | 1:13:A:GLY:HA3 | 1:12:A:VAL:H | 8 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 8 | 0.47 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 8 | 0.47 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 8 | 0.47 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 9 | 0.47 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 9 | 0.47 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 9 | 0.47 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 13 | 0.47 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 13 | 0.47 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 10 | 0.47 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 10 | 0.47 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 4 | 0.47 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 4 | 0.47 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 4 | 0.47 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 4 | 0.47 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 4 | 0.47 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 4 | 0.47 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 3 | 0.47 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 3 | 0.47 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 3 | 0.47 |
| (1,1754) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HA | 11 | 0.47 |
| (1,1754) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HA | 17 | 0.47 |
| (1,1754) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HA | 18 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD11 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD11 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD12 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD12 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD13 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD13 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD21 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD21 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD22 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD22 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD23 | 9 | 0.47 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD23 | 9 | 0.47 |
| (1,1405) | 1:29:A:ILE:HD11 | 1:32:A:ALA:HA | 13 | 0.47 |
| (1,3672) | 1:49:A:VAL:HG23 | 1:48:A:THR:H | 6 | 0.46 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 13 | 0.46 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 13 | 0.46 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 13 | 0.46 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 8 | 0.46 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 8 | 0.46 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 7 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 7 | 0.46 |
| (1,3368) | 1:48:A:THR:HG21 | 1:41:A:THR:H | 16 | 0.46 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 16 | 0.46 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 16 | 0.46 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 8 | 0.46 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 8 | 0.46 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 10 | 0.46 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 10 | 0.46 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 16 | 0.46 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 16 | 0.46 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG11 | 6 | 0.46 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG12 | 6 | 0.46 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG13 | 6 | 0.46 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG21 | 6 | 0.46 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG22 | 6 | 0.46 |
| (1,1735) | 1:93:A:PHE:HD1 | 1:92:A:VAL:HG23 | 6 | 0.46 |
| (1,1644) | 1:101:A:LEU:HD22 | 1:105:A:SER:HA | 20 | 0.46 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 10 | 0.46 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 10 | 0.46 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 14 | 0.46 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 14 | 0.46 |
| (1,1331) | 1:12:A:VAL:HG11 | 1:29:A:ILE:HA | 5 | 0.46 |
| (1,3680) | 1:19:A:LYS:HG3 | 1:24:A:PHE:H | 3 | 0.45 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 19 | 0.45 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 19 | 0.45 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 6 | 0.45 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 6 | 0.45 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 5 | 0.45 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 5 | 0.45 |
| (1,3585) | 1:84:A:THR:H | 1:36:A:VAL:HB | 6 | 0.45 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 9 | 0.45 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 9 | 0.45 |
| (1,3299) | 1:108:A:LEU:H | 1:10:A:LEU:HG | 13 | 0.45 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 7 | 0.45 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 7 | 0.45 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 14 | 0.45 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 14 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 8 | 0.45 |
| (1,1754) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HA | 10 | 0.45 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG11 | 2 | 0.45 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG12 | 2 | 0.45 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG13 | 2 | 0.45 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG21 | 2 | 0.45 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG22 | 2 | 0.45 |
| (1,1735) | 1:76:A:GLN:HE21 | 1:68:A:VAL:HG23 | 2 | 0.45 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG11 | 2 | 0.45 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG12 | 2 | 0.45 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG13 | 2 | 0.45 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG21 | 2 | 0.45 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG22 | 2 | 0.45 |
| (1,1692) | 1:41:A:THR:HG21 | 1:79:A:VAL:HG23 | 2 | 0.45 |
| (1,1629) | 1:91:A:VAL:HG23 | 1:93:A:PHE:HA | 20 | 0.45 |
| (1,1622) | 1:90:A:THR:HG22 | 1:30:A:LYS:HE2 | 15 | 0.45 |
| (1,1622) | 1:90:A:THR:HG22 | 1:30:A:LYS:HE3 | 15 | 0.45 |
| (1,1405) | 1:29:A:ILE:HD13 | 1:32:A:ALA:HA | 20 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1402) | 1:29:A:ILE:HD13 | 1:17:A:SER:H | 4 | 0.45 |
| (1,3666) | 1:39:A:LYS:HG2 | 1:41:A:THR:H | 8 | 0.44 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 4 | 0.44 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 6 | 0.44 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 6 | 0.44 |
| (1,3543) | 1:36:A:VAL:H | 1:85:A:ASP:HB2 | 1 | 0.44 |
| (1,3543) | 1:36:A:VAL:H | 1:85:A:ASP:HB3 | 1 | 0.44 |
| (1,3493) | 1:69:A:LYS:H | 1:42:A:PHE:HE1 | 19 | 0.44 |
| (1,3493) | 1:69:A:LYS:H | 1:42:A:PHE:HE2 | 19 | 0.44 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 18 | 0.44 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 18 | 0.44 |
| (1,3368) | 1:48:A:THR:HG22 | 1:41:A:THR:H | 19 | 0.44 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD11 | 1 | 0.44 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD12 | 1 | 0.44 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD13 | 1 | 0.44 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD21 | 1 | 0.44 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD22 | 1 | 0.44 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD23 | 1 | 0.44 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 2 | 0.44 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 2 | 0.44 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 17 | 0.44 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 17 | 0.44 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG2 | 17 | 0.44 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG3 | 17 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 2 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 2 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 13 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 1 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 4 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 5 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 9 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 13 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 18 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 1 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 1 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 5 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 7 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 17 | 0.44 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 10 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 1 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 4 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 5 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 7 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 17 | 0.44 |
| (1,1754) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HA | 1 | 0.44 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 20 | 0.44 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 20 | 0.44 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:29:A:ILE:HA | 10 | 0.44 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 9 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 1 | 0.43 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 1 | 0.43 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 16 | 0.43 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 16 | 0.43 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 16 | 0.43 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 16 | 0.43 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 16 | 0.43 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 16 | 0.43 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG21 | 1 | 0.43 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG22 | 1 | 0.43 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG23 | 1 | 0.43 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD11 | 15 | 0.43 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD12 | 15 | 0.43 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD13 | 15 | 0.43 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD21 | 15 | 0.43 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD22 | 15 | 0.43 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD23 | 15 | 0.43 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG2 | 8 | 0.43 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG3 | 8 | 0.43 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 13 | 0.43 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 13 | 0.43 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 13 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 6 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 10 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (\AA) |
|------------|----------------|----------------|-----------------|--|
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 12 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 14 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 15 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 16 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 17 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (\AA) |
|----------|----------------|-----------------|----------|----------------------------|
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 19 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 20 | 0.43 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG21 | 1 | 0.43 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG22 | 1 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG23 | 1 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 9 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 9 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 14 | 0.43 |
| (1,1754) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HA | 4 | 0.43 |
| (1,1754) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HA | 12 | 0.43 |
| (1,1754) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HA | 13 | 0.43 |
| (1,1500) | 1:56:A:ILE:HD12 | 1:55:A:HIS:HA | 14 | 0.43 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 15 | 0.43 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 15 | 0.43 |
| (1,3702) | 1:33:A:LYS:HE2 | 1:32:A:ALA:H | 14 | 0.42 |
| (1,3685) | 1:25:A:CYS:HB3 | 1:26:A:GLU:H | 6 | 0.42 |
| (1,3685) | 1:25:A:CYS:HB3 | 1:26:A:GLU:H | 7 | 0.42 |
| (1,3652) | 1:98:A:GLU:HB3 | 1:99:A:LYS:H | 16 | 0.42 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 9 | 0.42 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 9 | 0.42 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 17 | 0.42 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 17 | 0.42 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 12 | 0.42 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 12 | 0.42 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 2 | 0.42 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 2 | 0.42 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG2 | 4 | 0.42 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG3 | 4 | 0.42 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 6 | 0.42 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 6 | 0.42 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 6 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 10 | 0.42 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 10 | 0.42 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 10 | 0.42 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD2 | 11 | 0.42 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD3 | 11 | 0.42 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 1 | 0.42 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 6 | 0.42 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB2 | 12 | 0.42 |
| (1,1976) | 1:110:A:GLY:HA3 | 1:108:A:LEU:HB3 | 12 | 0.42 |
| (1,1947) | 1:40:A:VAL:HG11 | 1:79:A:VAL:HB | 10 | 0.42 |
| (1,1947) | 1:40:A:VAL:HG11 | 1:79:A:VAL:HB | 18 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1888) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 7 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 8 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG2 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD2 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1887) | 1:59:A:PRO:HG3 | 1:59:A:PRO:HD3 | 11 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 3 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 6 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 10 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 12 | 0.42 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 11 | 0.42 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 15 | 0.42 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 20 | 0.42 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 5 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 3 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 3 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 3 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 6 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 10 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 10 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 12 | 0.42 |
| (1,1754) | 1:51:A:VAL:HG23 | 1:53:A:ASP:HA | 6 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 1 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 1 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 4 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 4 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 5 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 5 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 7 | 0.42 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 7 | 0.42 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:32:A:ALA:HA | 2 | 0.42 |
| (1,3675) | 1:29:A:ILE:HG23 | 1:91:A:VAL:H | 20 | 0.41 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 2 | 0.41 |
| (1,3611) | 1:105:A:SER:HB3 | 1:19:A:LYS:H | 16 | 0.41 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 2 | 0.41 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 2 | 0.41 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 2 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 8 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 8 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 8 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 8 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 8 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 8 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 20 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 20 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 20 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 20 | 0.41 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 20 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 2 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 11 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 13 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 15 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 16 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 18 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 20 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 1 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 3 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 4 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 5 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 6 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 7 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 9 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 11 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 13 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 14 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 17 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 2 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 11 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 13 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 15 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 16 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 18 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 20 | 0.41 |
| (1,1754) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HA | 14 | 0.41 |
| (1,1419) | 1:100:A:THR:HG23 | 1:89:A:TYR:H | 14 | 0.41 |
| (1,3680) | 1:38:A:VAL:HG13 | 1:53:A:ASP:H | 17 | 0.4 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG2 | 15 | 0.4 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG3 | 15 | 0.4 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 17 | 0.4 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 17 | 0.4 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 17 | 0.4 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD21 | 7 | 0.4 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD22 | 7 | 0.4 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 6 | 0.4 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 6 | 0.4 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 6 | 0.4 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 6 | 0.4 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 6 | 0.4 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 6 | 0.4 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 11 | 0.4 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 11 | 0.4 |
| (1,3368) | 1:48:A:THR:HG21 | 1:41:A:THR:H | 5 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD11 | 10 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD12 | 10 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD13 | 10 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD21 | 10 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD22 | 10 | 0.4 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD23 | 10 | 0.4 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG2 | 19 | 0.4 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG3 | 19 | 0.4 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG2 | 11 | 0.4 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG3 | 11 | 0.4 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 20 | 0.4 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 20 | 0.4 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 20 | 0.4 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD2 | 13 | 0.4 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD3 | 13 | 0.4 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 15 | 0.4 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 8 | 0.4 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 8 | 0.4 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 8 | 0.4 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 8 | 0.4 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 8 | 0.4 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 8 | 0.4 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG21 | 6 | 0.4 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG22 | 6 | 0.4 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG23 | 6 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 8 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 12 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 16 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 16 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 19 | 0.4 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 2 | 0.4 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 6 | 0.4 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 6 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,3685) | 1:25:A:CYS:HB3 | 1:26:A:GLU:H | 20 | 0.39 |
| (1,3611) | 1:13:A:GLY:HA3 | 1:12:A:VAL:H | 14 | 0.39 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 2 | 0.39 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 2 | 0.39 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD11 | 3 | 0.39 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD12 | 3 | 0.39 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD13 | 3 | 0.39 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD21 | 3 | 0.39 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD22 | 3 | 0.39 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD23 | 3 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 1 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 1 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 1 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 1 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 1 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 1 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 12 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 12 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 12 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 12 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 12 | 0.39 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 12 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 19 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 19 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 19 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 19 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 19 | 0.39 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 19 | 0.39 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 8 | 0.39 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 13 | 0.39 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 17 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 4 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 12 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 4 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 12 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 14 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 10 | 0.39 |
| (1,1644) | 1:101:A:LEU:HD21 | 1:99:A:LYS:HA | 11 | 0.39 |
| (1,1629) | 1:91:A:VAL:HG22 | 1:99:A:LYS:HA | 6 | 0.39 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 12 | 0.39 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 12 | 0.39 |
| (1,1331) | 1:12:A:VAL:HG23 | 1:29:A:ILE:HA | 13 | 0.39 |
| (1,1331) | 1:12:A:VAL:HG11 | 1:29:A:ILE:HA | 20 | 0.39 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 10 | 0.38 |
| (1,3685) | 1:25:A:CYS:HB3 | 1:26:A:GLU:H | 1 | 0.38 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 16 | 0.38 |
| (1,3580) | 1:77:A:GLU:H | 1:44:A:HIS:HB2 | 2 | 0.38 |
| (1,3580) | 1:77:A:GLU:H | 1:44:A:HIS:HB3 | 2 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 6 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 6 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 6 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 6 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 6 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 6 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 12 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 12 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 12 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 12 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 12 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 12 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 13 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 13 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 13 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 13 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 13 | 0.38 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 13 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB2 | 4 | 0.38 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HB3 | 4 | 0.38 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 14 | 0.38 |
| (1,1947) | 1:40:A:VAL:HG12 | 1:79:A:VAL:HB | 2 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 5 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 6 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 9 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 11 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 15 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 5 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 6 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 9 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 11 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG23 | 20 | 0.38 |
| (1,3662) | 1:112:A:ARG:HB2 | 1:113:A:HIS:H | 10 | 0.37 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 11 | 0.37 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 11 | 0.37 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 11 | 0.37 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 11 | 0.37 |
| (1,3585) | 1:84:A:THR:H | 1:36:A:VAL:HB | 15 | 0.37 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 13 | 0.37 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 13 | 0.37 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 6 | 0.37 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 6 | 0.37 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 6 | 0.37 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 6 | 0.37 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 6 | 0.37 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 6 | 0.37 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 2 | 0.37 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 2 | 0.37 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 2 | 0.37 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 2 | 0.37 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 2 | 0.37 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 2 | 0.37 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 17 | 0.37 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 17 | 0.37 |
| (1,3218) | 1:36:A:VAL:H | 1:52:A:GLN:HB2 | 1 | 0.37 |
| (1,3218) | 1:36:A:VAL:H | 1:52:A:GLN:HB3 | 1 | 0.37 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 11 | 0.37 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 11 | 0.37 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 11 | 0.37 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 11 | 0.37 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 11 | 0.37 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 11 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 7 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 8 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 16 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 20 | 0.37 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 20 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 7 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 8 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 16 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 20 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 13 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 13 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 17 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 17 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 19 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 19 | 0.37 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 6 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:29:A:ILE:HG12 | 15 | 0.37 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:29:A:ILE:HG13 | 15 | 0.37 |
| (1,1405) | 1:29:A:ILE:HD11 | 1:32:A:ALA:HA | 4 | 0.37 |
| (1,1405) | 1:29:A:ILE:HD13 | 1:32:A:ALA:HA | 12 | 0.37 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:16:A:VAL:H | 14 | 0.37 |
| (1,1350) | 1:17:A:SER:HB3 | 1:16:A:VAL:HB | 12 | 0.37 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 16 | 0.36 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 16 | 0.36 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 16 | 0.36 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 11 | 0.36 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 11 | 0.36 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 16 | 0.36 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 16 | 0.36 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 5 | 0.36 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 5 | 0.36 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 19 | 0.36 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 19 | 0.36 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 17 | 0.36 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 17 | 0.36 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 17 | 0.36 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 17 | 0.36 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 17 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 17 | 0.36 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 6 | 0.36 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 6 | 0.36 |
| (1,3319) | 1:88:A:TRP:H | 1:33:A:LYS:HG2 | 18 | 0.36 |
| (1,3319) | 1:88:A:TRP:H | 1:33:A:LYS:HG3 | 18 | 0.36 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 8 | 0.36 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 8 | 0.36 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 8 | 0.36 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG2 | 13 | 0.36 |
| (1,3238) | 1:79:A:VAL:H | 1:77:A:GLU:HG3 | 13 | 0.36 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 12 | 0.36 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 12 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 10 | 0.36 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 10 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 10 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 17 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 17 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 9 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 9 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HD3 | 19 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD2 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1848) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HD3 | 19 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 18 | 0.36 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 17 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG2 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1761) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HG3 | 19 | 0.36 |
| (1,1629) | 1:91:A:VAL:HG23 | 1:99:A:LYS:HA | 12 | 0.36 |
| (1,1419) | 1:100:A:THR:HG21 | 1:89:A:TYR:H | 5 | 0.36 |
| (1,3672) | 1:41:A:THR:HG23 | 1:48:A:THR:H | 10 | 0.35 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 6 | 0.35 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 9 | 0.35 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 6 | 0.35 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 6 | 0.35 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 18 | 0.35 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 18 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG11 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG11 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG12 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG12 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG13 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG13 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG21 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG21 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG22 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG22 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG23 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG23 | 3 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG11 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG11 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG12 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG12 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG13 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG13 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG21 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG22 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG22 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG23 | 13 | 0.35 |
| (1,3406) | 1:55:A:HIS:H | 1:38:A:VAL:HG23 | 13 | 0.35 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 8 | 0.35 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 8 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG2 | 12 | 0.35 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG3 | 12 | 0.35 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 4 | 0.35 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 4 | 0.35 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 7 | 0.35 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 7 | 0.35 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 7 | 0.35 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 20 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 6 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 6 | 0.35 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 18 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 2 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 15 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 15 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD2 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG2 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1847) | 1:142:A:ARG:HD3 | 1:142:A:ARG:HG3 | 20 | 0.35 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 18 | 0.35 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 19 | 0.35 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG2 | 4 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG3 | 4 | 0.35 |
| (1,1486) | 1:50:A:GLU:HG3 | 1:37:A:LYS:HA | 13 | 0.35 |
| (1,1382) | 1:27:A:ALA:HB3 | 1:26:A:GLU:HB2 | 1 | 0.35 |
| (1,1382) | 1:27:A:ALA:HB3 | 1:26:A:GLU:HB3 | 1 | 0.35 |
| (1,1331) | 1:12:A:VAL:HG21 | 1:31:A:THR:HB | 16 | 0.35 |
| (1,3666) | 1:39:A:LYS:HG2 | 1:41:A:THR:H | 3 | 0.34 |
| (1,3652) | 1:98:A:GLU:HB3 | 1:99:A:LYS:H | 1 | 0.34 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 5 | 0.34 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 5 | 0.34 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 5 | 0.34 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 5 | 0.34 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 5 | 0.34 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 11 | 0.34 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 11 | 0.34 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 11 | 0.34 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 11 | 0.34 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 11 | 0.34 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 11 | 0.34 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG11 | 10 | 0.34 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG12 | 10 | 0.34 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG13 | 10 | 0.34 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG21 | 10 | 0.34 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG22 | 10 | 0.34 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG23 | 10 | 0.34 |
| (1,3368) | 1:48:A:THR:HG22 | 1:41:A:THR:H | 2 | 0.34 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG21 | 17 | 0.34 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG22 | 17 | 0.34 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG23 | 17 | 0.34 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG2 | 13 | 0.34 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG3 | 13 | 0.34 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 9 | 0.34 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 9 | 0.34 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 3 | 0.34 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 9 | 0.34 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 10 | 0.34 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 10 | 0.34 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 10 | 0.34 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 10 | 0.34 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 10 | 0.34 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 10 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 20 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 20 | 0.34 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB1 | 11 | 0.34 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB2 | 11 | 0.34 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB3 | 11 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 1 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 2 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 3 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 13 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1878) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 1 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 2 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 3 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 13 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 19 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 6 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 6 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 8 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 8 | 0.34 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 4 | 0.34 |
| (1,1629) | 1:91:A:VAL:HG21 | 1:93:A:PHE:HA | 17 | 0.34 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 5 | 0.34 |
| (1,1500) | 1:56:A:ILE:HD13 | 1:55:A:HIS:HA | 10 | 0.34 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 2 | 0.34 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 2 | 0.34 |
| (1,1331) | 1:12:A:VAL:HG11 | 1:29:A:ILE:HA | 18 | 0.34 |
| (1,3611) | 1:13:A:GLY:HA3 | 1:12:A:VAL:H | 18 | 0.33 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 12 | 0.33 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 12 | 0.33 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 4 | 0.33 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 4 | 0.33 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 10 | 0.33 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 10 | 0.33 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD21 | 12 | 0.33 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD22 | 12 | 0.33 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG21 | 13 | 0.33 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG22 | 13 | 0.33 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG23 | 13 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 13 | 0.33 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 13 | 0.33 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 18 | 0.33 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 19 | 0.33 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 19 | 0.33 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 19 | 0.33 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 19 | 0.33 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 19 | 0.33 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 19 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA2 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD3 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |
| (1,1886) | 1:58:A:GLY:HA3 | 1:59:A:PRO:HD2 | 18 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD2 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA2 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1877) | 1:59:A:PRO:HD3 | 1:58:A:GLY:HA3 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 12 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 12 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 18 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 16 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 20 | 0.33 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB2 | 7 | 0.33 |
| (1,1622) | 1:90:A:THR:HG23 | 1:88:A:TRP:HB3 | 7 | 0.33 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG11 | 15 | 0.33 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG12 | 15 | 0.33 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG13 | 15 | 0.33 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG21 | 15 | 0.33 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG22 | 15 | 0.33 |
| (1,1484) | 1:50:A:GLU:HA | 1:51:A:VAL:HG23 | 15 | 0.33 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:32:A:ALA:HA | 11 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3685) | 1:25:A:CYS:HB3 | 1:26:A:GLU:H | 5 | 0.32 |
| (1,3672) | 1:41:A:THR:HG21 | 1:48:A:THR:H | 9 | 0.32 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 12 | 0.32 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 12 | 0.32 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG2 | 12 | 0.32 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG3 | 12 | 0.32 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 18 | 0.32 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 18 | 0.32 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 18 | 0.32 |
| (1,3267) | 1:111:A:GLU:H | 1:112:A:ARG:HB2 | 2 | 0.32 |
| (1,3267) | 1:111:A:GLU:H | 1:112:A:ARG:HB2 | 2 | 0.32 |
| (1,3267) | 1:111:A:GLU:H | 1:112:A:ARG:HB3 | 2 | 0.32 |
| (1,3267) | 1:111:A:GLU:H | 1:112:A:ARG:HB3 | 2 | 0.32 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 18 | 0.32 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 18 | 0.32 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 5 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 3 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 11 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 11 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 3 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 3 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 16 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 16 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 9 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 8 | 0.32 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD1 | 6 | 0.32 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD2 | 6 | 0.32 |
| (1,3680) | 1:38:A:VAL:HG12 | 1:53:A:ASP:H | 13 | 0.31 |
| (1,3611) | 1:105:A:SER:HB3 | 1:19:A:LYS:H | 7 | 0.31 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 12 | 0.31 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 12 | 0.31 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 12 | 0.31 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 12 | 0.31 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 12 | 0.31 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD1 | 19 | 0.31 |
| (1,3587) | 1:88:A:TRP:H | 1:89:A:TYR:HD2 | 19 | 0.31 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 16 | 0.31 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 16 | 0.31 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 4 | 0.31 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 4 | 0.31 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG2 | 12 | 0.31 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG3 | 12 | 0.31 |
| (1,3312) | 1:3:A:ALA:HB1 | 1:4:A:LEU:H | 9 | 0.31 |
| (1,3299) | 1:108:A:LEU:H | 1:10:A:LEU:HG | 14 | 0.31 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 11 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 9 | 0.31 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 9 | 0.31 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 17 | 0.31 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 17 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 7 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 7 | 0.31 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 7 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 2 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 2 | 0.31 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG2 | 19 | 0.31 |
| (1,1819) | 1:57:A:LYS:HD3 | 1:67:A:GLU:HG3 | 19 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 12 | 0.31 |
| (1,956) | 1:98:A:GLU:HG2 | 1:92:A:VAL:HB | 13 | 0.31 |
| (1,956) | 1:98:A:GLU:HG3 | 1:92:A:VAL:HB | 13 | 0.31 |
| (1,3714) | 1:115:A:ALA:HB1 | 1:114:A:PHE:H | 2 | 0.3 |
| (1,3709) | 1:66:A:VAL:HG11 | 1:58:A:GLY:H | 18 | 0.3 |
| (1,3681) | 1:66:A:VAL:HG11 | 1:58:A:GLY:H | 18 | 0.3 |
| (1,3672) | 1:41:A:THR:HG22 | 1:48:A:THR:H | 3 | 0.3 |
| (1,3662) | 1:120:A:LEU:HB3 | 1:121:A:ASP:H | 4 | 0.3 |
| (1,3652) | 1:98:A:GLU:HB3 | 1:99:A:LYS:H | 12 | 0.3 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 15 | 0.3 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 15 | 0.3 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 15 | 0.3 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 20 | 0.3 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 20 | 0.3 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 1 | 0.3 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 1 | 0.3 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 14 | 0.3 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 14 | 0.3 |
| (1,3541) | 1:38:A:VAL:H | 1:37:A:LYS:HE2 | 13 | 0.3 |
| (1,3541) | 1:38:A:VAL:H | 1:37:A:LYS:HE3 | 13 | 0.3 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 17 | 0.3 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 17 | 0.3 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 17 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 8 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 8 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 8 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 8 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 8 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 8 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 18 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 18 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 18 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 18 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 18 | 0.3 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 18 | 0.3 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG2 | 7 | 0.3 |
| (1,3396) | 1:76:A:GLN:H | 1:69:A:LYS:HG3 | 7 | 0.3 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD11 | 14 | 0.3 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD12 | 14 | 0.3 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD13 | 14 | 0.3 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD21 | 14 | 0.3 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD22 | 14 | 0.3 |
| (1,3359) | 1:55:A:HIS:H | 1:60:A:LEU:HD23 | 14 | 0.3 |
| (1,3330) | 1:16:A:VAL:H | 1:28:A:LYS:HG2 | 12 | 0.3 |
| (1,3330) | 1:16:A:VAL:H | 1:28:A:LYS:HG3 | 12 | 0.3 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 12 | 0.3 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 12 | 0.3 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 2 | 0.3 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 2 | 0.3 |
| (1,3214) | 1:57:A:LYS:H | 1:66:A:VAL:HB | 13 | 0.3 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 13 | 0.3 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 13 | 0.3 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 6 | 0.3 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 6 | 0.3 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 6 | 0.3 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 6 | 0.3 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 6 | 0.3 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 2 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 4 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 4 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 6 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG11 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG11 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG12 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG12 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG13 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG13 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG21 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG21 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG22 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG22 | 18 | 0.3 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG23 | 18 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1405) | 1:29:A:ILE:HD11 | 1:32:A:ALA:HA | 9 | 0.3 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 19 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 19 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 19 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 20 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 20 | 0.29 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 20 | 0.29 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB2 | 16 | 0.29 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB3 | 16 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 17 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 17 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 17 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 17 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 17 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 17 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 19 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 19 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 19 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 19 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 19 | 0.29 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 19 | 0.29 |
| (1,3354) | 1:49:A:VAL:H | 1:39:A:LYS:HG2 | 20 | 0.29 |
| (1,3354) | 1:49:A:VAL:H | 1:39:A:LYS:HG3 | 20 | 0.29 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG2 | 16 | 0.29 |
| (1,3340) | 1:88:A:TRP:HE1 | 1:102:A:ARG:HG3 | 16 | 0.29 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG2 | 7 | 0.29 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG3 | 7 | 0.29 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 18 | 0.29 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 18 | 0.29 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG2 | 12 | 0.29 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG3 | 12 | 0.29 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD2 | 15 | 0.29 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD3 | 15 | 0.29 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB2 | 15 | 0.29 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB3 | 15 | 0.29 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 7 | 0.29 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 7 | 0.29 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 10 | 0.29 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 2 | 0.29 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 9 | 0.29 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 11 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 17 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 17 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 17 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 17 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 17 | 0.29 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 12 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 17 | 0.29 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 14 | 0.29 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 16 | 0.29 |
| (1,1819) | 1:28:A:LYS:HG3 | 1:29:A:ILE:HB | 7 | 0.29 |
| (1,1539) | 1:65:A:ILE:HD12 | 1:80:A:ILE:H | 14 | 0.29 |
| (1,1419) | 1:100:A:THR:HG21 | 1:89:A:TYR:H | 4 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1419) | 1:100:A:THR:HG21 | 1:89:A:TYR:H | 6 | 0.29 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD1 | 4 | 0.29 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD2 | 4 | 0.29 |
| (1,3652) | 1:98:A:GLU:HB3 | 1:99:A:LYS:H | 13 | 0.28 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 1 | 0.28 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 4 | 0.28 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 7 | 0.28 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 7 | 0.28 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 7 | 0.28 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG11 | 15 | 0.28 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG12 | 15 | 0.28 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG13 | 15 | 0.28 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG21 | 15 | 0.28 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG22 | 15 | 0.28 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG23 | 15 | 0.28 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG21 | 6 | 0.28 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG22 | 6 | 0.28 |
| (1,3354) | 1:49:A:VAL:H | 1:48:A:THR:HG23 | 6 | 0.28 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG2 | 20 | 0.28 |
| (1,3332) | 1:13:A:GLY:H | 1:28:A:LYS:HG3 | 20 | 0.28 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 19 | 0.28 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 19 | 0.28 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HD2 | 4 | 0.28 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HD3 | 4 | 0.28 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 14 | 0.28 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 14 | 0.28 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 15 | 0.28 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 15 | 0.28 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 15 | 0.28 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 15 | 0.28 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 15 | 0.28 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 15 | 0.28 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 15 | 0.28 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 8 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 8 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 15 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 7 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 7 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 11 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 11 | 0.28 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG21 | 18 | 0.28 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG22 | 18 | 0.28 |
| (1,1855) | 1:83:A:LEU:HA | 1:84:A:THR:HG23 | 18 | 0.28 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 12 | 0.28 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 4 | 0.28 |
| (1,1500) | 1:56:A:ILE:HD13 | 1:55:A:HIS:HA | 6 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3662) | 1:120:A:LEU:HB3 | 1:121:A:ASP:H | 14 | 0.27 |
| (1,3638) | 1:52:A:GLN:HG3 | 1:52:A:GLN:H | 15 | 0.27 |
| (1,3623) | 1:35:A:LEU:HA | 1:53:A:ASP:H | 20 | 0.27 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 18 | 0.27 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 18 | 0.27 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 19 | 0.27 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 19 | 0.27 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 5 | 0.27 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 5 | 0.27 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD21 | 5 | 0.27 |
| (1,3493) | 1:69:A:LYS:H | 1:70:A:ASN:HD22 | 5 | 0.27 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 9 | 0.27 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 9 | 0.27 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 9 | 0.27 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 13 | 0.27 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 13 | 0.27 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 13 | 0.27 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 18 | 0.27 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 18 | 0.27 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 18 | 0.27 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 18 | 0.27 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 18 | 0.27 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 18 | 0.27 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 6 | 0.27 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 6 | 0.27 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 18 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 14 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 14 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 5 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 5 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 10 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 9 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 9 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 13 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 19 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 19 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 19 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 20 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 15 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 15 | 0.27 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 11 | 0.27 |
| (1,1677) | 1:33:A:LYS:HB3 | 1:35:A:LEU:HG | 20 | 0.27 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 20 | 0.27 |
| (1,3702) | 1:24:A:PHE:HB3 | 1:20:A:TYR:H | 5 | 0.26 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 11 | 0.26 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 11 | 0.26 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 11 | 0.26 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB1 | 10 | 0.26 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB2 | 10 | 0.26 |
| (1,3591) | 1:89:A:TYR:H | 1:32:A:ALA:HB3 | 10 | 0.26 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 1 | 0.26 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 1 | 0.26 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 11 | 0.26 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 11 | 0.26 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 19 | 0.26 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 19 | 0.26 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 3 | 0.26 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 3 | 0.26 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 3 | 0.26 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 19 | 0.26 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 19 | 0.26 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 19 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 2 | 0.26 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 2 | 0.26 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 2 | 0.26 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 2 | 0.26 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 2 | 0.26 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 2 | 0.26 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 3 | 0.26 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 3 | 0.26 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 3 | 0.26 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 3 | 0.26 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 3 | 0.26 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 3 | 0.26 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 3 | 0.26 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 3 | 0.26 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 3 | 0.26 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 3 | 0.26 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 3 | 0.26 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 3 | 0.26 |
| (1,3368) | 1:48:A:THR:HG21 | 1:41:A:THR:H | 15 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 3 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 3 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 10 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 10 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 16 | 0.26 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 16 | 0.26 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 7 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 14 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 14 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 1 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 10 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 14 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 1 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 1 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 2 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 3 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 6 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 6 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 9 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 9 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 9 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 14 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 14 | 0.26 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB1 | 20 | 0.26 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB2 | 20 | 0.26 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB3 | 20 | 0.26 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 9 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 17 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 17 | 0.26 |
| (1,1629) | 1:91:A:VAL:HG21 | 1:99:A:LYS:HA | 8 | 0.26 |
| (1,1419) | 1:100:A:THR:HG22 | 1:89:A:TYR:H | 10 | 0.26 |
| (1,3671) | 1:65:A:ILE:HG12 | 1:66:A:VAL:H | 13 | 0.25 |
| (1,3649) | 1:98:A:GLU:HB3 | 1:91:A:VAL:H | 3 | 0.25 |
| (1,3642) | 1:66:A:VAL:HB | 1:58:A:GLY:H | 1 | 0.25 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 19 | 0.25 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 11 | 0.25 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 12 | 0.25 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 12 | 0.25 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB2 | 8 | 0.25 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB3 | 8 | 0.25 |
| (1,3415) | 1:63:A:GLY:H | 1:79:A:VAL:HG11 | 7 | 0.25 |
| (1,3415) | 1:63:A:GLY:H | 1:79:A:VAL:HG12 | 7 | 0.25 |
| (1,3415) | 1:63:A:GLY:H | 1:79:A:VAL:HG13 | 7 | 0.25 |
| (1,3415) | 1:63:A:GLY:H | 1:79:A:VAL:HG21 | 7 | 0.25 |
| (1,3415) | 1:63:A:GLY:H | 1:79:A:VAL:HG22 | 7 | 0.25 |
| (1,3415) | 1:63:A:GLY:H | 1:79:A:VAL:HG23 | 7 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 2 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 2 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 2 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 8 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 8 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 8 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 16 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 16 | 0.25 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 16 | 0.25 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 19 | 0.25 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 19 | 0.25 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 19 | 0.25 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 19 | 0.25 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 19 | 0.25 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 19 | 0.25 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 4 | 0.25 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 18 | 0.25 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 18 | 0.25 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 18 | 0.25 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 18 | 0.25 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 18 | 0.25 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 5 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 5 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 8 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 8 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 10 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 10 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 12 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 12 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 13 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 15 | 0.25 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 15 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 17 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 17 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 18 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 18 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 3 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 1 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 1 | 0.25 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 1 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 1 | 0.25 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 9 | 0.25 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 9 | 0.25 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:31:A:THR:HB | 3 | 0.25 |
| (1,59) | 1:93:A:PHE:HD2 | 1:91:A:VAL:HB | 13 | 0.25 |
| (1,59) | 1:93:A:PHE:HD1 | 1:91:A:VAL:HB | 18 | 0.25 |
| (1,3671) | 1:65:A:ILE:HG12 | 1:66:A:VAL:H | 18 | 0.24 |
| (1,3641) | 1:67:A:GLU:HB2 | 1:58:A:GLY:H | 18 | 0.24 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 14 | 0.24 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 14 | 0.24 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 3 | 0.24 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 3 | 0.24 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 18 | 0.24 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 18 | 0.24 |
| (1,3542) | 1:85:A:ASP:H | 1:83:A:LEU:HB2 | 6 | 0.24 |
| (1,3542) | 1:85:A:ASP:H | 1:83:A:LEU:HB3 | 6 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 1 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 1 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 1 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 15 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 15 | 0.24 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 15 | 0.24 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 9 | 0.24 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 9 | 0.24 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 9 | 0.24 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 9 | 0.24 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 9 | 0.24 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 9 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 7 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 7 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 7 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 7 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 7 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 7 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG11 | 14 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG12 | 14 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG13 | 14 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG21 | 14 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG22 | 14 | 0.24 |
| (1,3389) | 1:64:A:ALA:H | 1:79:A:VAL:HG23 | 14 | 0.24 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 2 | 0.24 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 2 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 2 | 0.24 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 10 | 0.24 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 10 | 0.24 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 10 | 0.24 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 7 | 0.24 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 7 | 0.24 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 9 | 0.24 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 9 | 0.24 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 9 | 0.24 |
| (1,3258) | 1:109:A:LYS:H | 1:109:A:LYS:HB2 | 3 | 0.24 |
| (1,3258) | 1:109:A:LYS:H | 1:109:A:LYS:HB3 | 3 | 0.24 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 4 | 0.24 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 4 | 0.24 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 3 | 0.24 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 14 | 0.24 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 3 | 0.24 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 3 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 6 | 0.24 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 2 | 0.24 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 2 | 0.24 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 2 | 0.24 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 2 | 0.24 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 2 | 0.24 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 2 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 16 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 16 | 0.24 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 4 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 16 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1912) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD21 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD22 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB2 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1912) | 1:71:A:LEU:HD23 | 1:71:A:LEU:HB3 | 16 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 1 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 2 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 2 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 4 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 5 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 5 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 9 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 10 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 13 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 13 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 18 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 19 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 19 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 20 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 11 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 11 | 0.24 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 15 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 10 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 19 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 19 | 0.24 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 7 | 0.24 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:32:A:ALA:HA | 16 | 0.24 |
| (1,3664) | 1:101:A:LEU:HD22 | 1:106:A:LEU:H | 20 | 0.23 |
| (1,3633) | 1:76:A:GLN:HB3 | 1:77:A:GLU:H | 1 | 0.23 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 10 | 0.23 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 10 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 6 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 6 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 6 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 7 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 7 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 7 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 10 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 10 | 0.23 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 10 | 0.23 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 16 | 0.23 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 16 | 0.23 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 16 | 0.23 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 16 | 0.23 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 16 | 0.23 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 16 | 0.23 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG2 | 9 | 0.23 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG3 | 9 | 0.23 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG2 | 18 | 0.23 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG3 | 18 | 0.23 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 17 | 0.23 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 17 | 0.23 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG2 | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG3 | 3 | 0.23 |
| (1,3299) | 1:108:A:LEU:H | 1:10:A:LEU:HG | 1 | 0.23 |
| (1,3299) | 1:108:A:LEU:H | 1:10:A:LEU:HG | 3 | 0.23 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 19 | 0.23 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 19 | 0.23 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 16 | 0.23 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 19 | 0.23 |
| (1,2447) | 1:99:A:LYS:HG2 | 1:98:A:GLU:H | 6 | 0.23 |
| (1,2447) | 1:99:A:LYS:HG3 | 1:98:A:GLU:H | 6 | 0.23 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 4 | 0.23 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 4 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 6 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 11 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 11 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 12 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 14 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 15 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 15 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 16 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 17 | 0.23 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 7 | 0.23 |
| (1,1677) | 1:33:A:LYS:HB3 | 1:35:A:LEU:HG | 6 | 0.23 |
| (1,1629) | 1:91:A:VAL:HG22 | 1:27:A:ALA:HA | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1405) | 1:29:A:ILE:HD11 | 1:32:A:ALA:HA | 5 | 0.23 |
| (1,1401) | 1:29:A:ILE:HD13 | 1:16:A:VAL:H | 13 | 0.23 |
| (1,1315) | 1:115:A:ALA:HA | 1:114:A:PHE:H | 1 | 0.23 |
| (1,1315) | 1:115:A:ALA:HA | 1:114:A:PHE:H | 12 | 0.23 |
| (1,3671) | 1:65:A:ILE:HG12 | 1:66:A:VAL:H | 17 | 0.22 |
| (1,3614) | 1:113:A:HIS:HA | 1:114:A:PHE:H | 1 | 0.22 |
| (1,3541) | 1:38:A:VAL:H | 1:37:A:LYS:HE2 | 9 | 0.22 |
| (1,3541) | 1:38:A:VAL:H | 1:37:A:LYS:HE3 | 9 | 0.22 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 17 | 0.22 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 17 | 0.22 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 20 | 0.22 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 20 | 0.22 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 12 | 0.22 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 12 | 0.22 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 12 | 0.22 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 4 | 0.22 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 4 | 0.22 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 4 | 0.22 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 4 | 0.22 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 4 | 0.22 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 4 | 0.22 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG2 | 8 | 0.22 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG3 | 8 | 0.22 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG2 | 15 | 0.22 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG3 | 15 | 0.22 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 16 | 0.22 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 16 | 0.22 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 2 | 0.22 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 2 | 0.22 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 2 | 0.22 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 8 | 0.22 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 8 | 0.22 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 14 | 0.22 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 14 | 0.22 |
| (1,3217) | 1:38:A:VAL:H | 1:38:A:VAL:HB | 18 | 0.22 |
| (1,3214) | 1:57:A:LYS:H | 1:66:A:VAL:HB | 7 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 10 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 10 | 0.22 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 10 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 12 | 0.22 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 20 | 0.22 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 20 | 0.22 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 20 | 0.22 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 20 | 0.22 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 20 | 0.22 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 20 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 7 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 7 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD2 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG2 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1882) | 1:59:A:PRO:HD3 | 1:59:A:PRO:HG3 | 8 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 10 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 1 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 1 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 15 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 19 | 0.22 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 19 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG2 | 9 | 0.22 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG3 | 9 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 1 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 1 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 14 | 0.22 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 11 | 0.22 |
| (1,956) | 1:98:A:GLU:HG2 | 1:92:A:VAL:HB | 8 | 0.22 |
| (1,956) | 1:98:A:GLU:HG3 | 1:92:A:VAL:HB | 8 | 0.22 |
| (1,3673) | 1:35:A:LEU:HD11 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD11 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD11 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD11 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD12 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD12 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD12 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD12 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD13 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD13 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD13 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD13 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD21 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD21 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD21 | 1:52:A:GLN:HE22 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3673) | 1:35:A:LEU:HD21 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD22 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD22 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD22 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD22 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD23 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD23 | 1:52:A:GLN:HE21 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD23 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3673) | 1:35:A:LEU:HD23 | 1:52:A:GLN:HE22 | 1 | 0.21 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 13 | 0.21 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG2 | 4 | 0.21 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG3 | 4 | 0.21 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 6 | 0.21 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 6 | 0.21 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 6 | 0.21 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 11 | 0.21 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 11 | 0.21 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 11 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 5 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 5 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 5 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 5 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 5 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 5 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 11 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 11 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 11 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 11 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 11 | 0.21 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 11 | 0.21 |
| (1,3368) | 1:48:A:THR:HG23 | 1:41:A:THR:H | 12 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 3 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 3 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 3 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 14 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 14 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 14 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 15 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 15 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 15 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 18 | 0.21 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 18 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 18 | 0.21 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HD2 | 11 | 0.21 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HD3 | 11 | 0.21 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG2 | 15 | 0.21 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG3 | 15 | 0.21 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB1 | 16 | 0.21 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB2 | 16 | 0.21 |
| (1,3294) | 1:34:A:ARG:H | 1:32:A:ALA:HB3 | 16 | 0.21 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 11 | 0.21 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 11 | 0.21 |
| (1,3183) | 1:67:A:GLU:H | 1:57:A:LYS:HA | 13 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 10 | 0.21 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 13 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 2 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 16 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 16 | 0.21 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 16 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 20 | 0.21 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 9 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 3 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 20 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 2 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 3 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 10 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 17 | 0.21 |
| (1,1629) | 1:91:A:VAL:HG22 | 1:93:A:PHE:HA | 14 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG11 | 2 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG12 | 2 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG13 | 2 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG21 | 2 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG22 | 2 | 0.21 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG23 | 2 | 0.21 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:31:A:THR:HB | 8 | 0.21 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG2 | 2 | 0.21 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG3 | 2 | 0.21 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG2 | 8 | 0.21 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG3 | 8 | 0.21 |
| (1,770) | 1:60:A:LEU:HG | 1:59:A:PRO:HA | 2 | 0.21 |
| (1,3614) | 1:5:A:ASP:HA | 1:6:A:GLU:H | 8 | 0.2 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 14 | 0.2 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 14 | 0.2 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 12 | 0.2 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 12 | 0.2 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 1 | 0.2 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 1 | 0.2 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 11 | 0.2 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 11 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD11 | 16 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD12 | 16 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD13 | 16 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD21 | 16 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD22 | 16 | 0.2 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD23 | 16 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 4 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 4 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 4 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 14 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 14 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 14 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 18 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 18 | 0.2 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 18 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 17 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 17 | 0.2 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 17 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 5 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 5 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 5 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 7 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 7 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 7 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 12 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 12 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 12 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 16 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 16 | 0.2 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 16 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 3 | 0.2 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 3 | 0.2 |
| (1,3330) | 1:16:A:VAL:H | 1:109:A:LYS:HG2 | 4 | 0.2 |
| (1,3330) | 1:16:A:VAL:H | 1:109:A:LYS:HG3 | 4 | 0.2 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG2 | 6 | 0.2 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG3 | 6 | 0.2 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 13 | 0.2 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 13 | 0.2 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG2 | 5 | 0.2 |
| (1,3313) | 1:40:A:VAL:H | 1:39:A:LYS:HG3 | 5 | 0.2 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB2 | 9 | 0.2 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB3 | 9 | 0.2 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 9 | 0.2 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 9 | 0.2 |
| (1,3214) | 1:57:A:LYS:H | 1:66:A:VAL:HB | 6 | 0.2 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 13 | 0.2 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 19 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 7 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG11 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG12 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG13 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG21 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG22 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 7 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE2 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1983) | 1:92:A:VAL:HG23 | 1:30:A:LYS:HE3 | 7 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 19 | 0.2 |
| (1,1947) | 1:91:A:VAL:HG12 | 1:30:A:LYS:HB2 | 20 | 0.2 |
| (1,1947) | 1:91:A:VAL:HG12 | 1:30:A:LYS:HB3 | 20 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 9 | 0.2 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 9 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 1 | 0.2 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 6 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 18 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 6 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 7 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 10 | 0.2 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 1 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 13 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 12 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 13 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 13 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 17 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 19 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 19 | 0.2 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 19 | 0.2 |
| (1,1331) | 1:12:A:VAL:HG23 | 1:29:A:ILE:HA | 15 | 0.2 |
| (1,770) | 1:60:A:LEU:HG | 1:59:A:PRO:HA | 8 | 0.2 |
| (1,3671) | 1:65:A:ILE:HG12 | 1:66:A:VAL:H | 6 | 0.19 |
| (1,3662) | 1:112:A:ARG:HB3 | 1:113:A:HIS:H | 1 | 0.19 |
| (1,3640) | 1:81:A:ASN:HB2 | 1:41:A:THR:H | 18 | 0.19 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 9 | 0.19 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB2 | 13 | 0.19 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB3 | 13 | 0.19 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 5 | 0.19 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 5 | 0.19 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 5 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 7 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 7 | 0.19 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 7 | 0.19 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 12 | 0.19 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 12 | 0.19 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 12 | 0.19 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD11 | 16 | 0.19 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD12 | 16 | 0.19 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD13 | 16 | 0.19 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD21 | 16 | 0.19 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD22 | 16 | 0.19 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD23 | 16 | 0.19 |
| (1,3322) | 1:54:A:ASP:H | 1:56:A:ILE:HG12 | 17 | 0.19 |
| (1,3322) | 1:54:A:ASP:H | 1:56:A:ILE:HG13 | 17 | 0.19 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG2 | 3 | 0.19 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG3 | 3 | 0.19 |
| (1,3158) | 1:118:A:GLU:H | 1:117:A:SER:HB2 | 11 | 0.19 |
| (1,3158) | 1:118:A:GLU:H | 1:117:A:SER:HB2 | 11 | 0.19 |
| (1,3158) | 1:118:A:GLU:H | 1:117:A:SER:HB3 | 11 | 0.19 |
| (1,3158) | 1:118:A:GLU:H | 1:117:A:SER:HB3 | 11 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 17 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD11 | 1:83:A:LEU:HB2 | 11 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1934) | 1:83:A:LEU:HD11 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD11 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD11 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD11 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD11 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD12 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD12 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD12 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD12 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD12 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD12 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD13 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD13 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD13 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD13 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD13 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD13 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD21 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD21 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD21 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD21 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD21 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD21 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD22 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD22 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD22 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD22 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD22 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD22 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD23 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD23 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD23 | 1:83:A:LEU:HB2 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD23 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1934) | 1:83:A:LEU:HD23 | 1:83:A:LEU:HB3 | 11 | 0.19 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG11 | 13 | 0.19 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG12 | 13 | 0.19 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG13 | 13 | 0.19 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG21 | 13 | 0.19 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG22 | 13 | 0.19 |
| (1,1929) | 1:65:A:ILE:HG12 | 1:79:A:VAL:HG23 | 13 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB2 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB2 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB2 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1919) | 1:67:A:GLU:HB3 | 1:75:A:TYR:HB3 | 18 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 5 | 0.19 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 10 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 1 | 0.19 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 2 | 0.19 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 4 | 0.19 |
| (1,1822) | 1:52:A:GLN:H | 1:38:A:VAL:HG11 | 4 | 0.19 |
| (1,1822) | 1:52:A:GLN:H | 1:38:A:VAL:HG12 | 4 | 0.19 |
| (1,1822) | 1:52:A:GLN:H | 1:38:A:VAL:HG13 | 4 | 0.19 |
| (1,1822) | 1:52:A:GLN:H | 1:38:A:VAL:HG21 | 4 | 0.19 |
| (1,1822) | 1:52:A:GLN:H | 1:38:A:VAL:HG22 | 4 | 0.19 |
| (1,1822) | 1:52:A:GLN:H | 1:38:A:VAL:HG23 | 4 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 2 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 2 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 5 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 18 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.19 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 18 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 13 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 9 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 9 | 0.19 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 9 | 0.19 |
| (1,1405) | 1:29:A:ILE:HD12 | 1:32:A:ALA:HA | 1 | 0.19 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG2 | 12 | 0.19 |
| (1,1277) | 1:108:A:LEU:HA | 1:109:A:LYS:HG3 | 12 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE2 | 9 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE3 | 9 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE2 | 9 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE3 | 9 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE2 | 16 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE3 | 16 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE2 | 16 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE3 | 16 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE2 | 19 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB2 | 1:37:A:LYS:HE3 | 19 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE2 | 19 | 0.19 |
| (1,1120) | 1:37:A:LYS:HB3 | 1:37:A:LYS:HE3 | 19 | 0.19 |
| (1,956) | 1:98:A:GLU:HG2 | 1:92:A:VAL:HB | 3 | 0.19 |
| (1,956) | 1:98:A:GLU:HG3 | 1:92:A:VAL:HB | 3 | 0.19 |
| (1,770) | 1:60:A:LEU:HG | 1:59:A:PRO:HA | 1 | 0.19 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 2 | 0.19 |
| (1,3642) | 1:66:A:VAL:HB | 1:58:A:GLY:H | 18 | 0.18 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB2 | 16 | 0.18 |
| (1,3558) | 1:30:A:LYS:H | 1:28:A:LYS:HB3 | 16 | 0.18 |
| (1,3543) | 1:36:A:VAL:H | 1:85:A:ASP:HB2 | 9 | 0.18 |
| (1,3543) | 1:36:A:VAL:H | 1:85:A:ASP:HB3 | 9 | 0.18 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 3 | 0.18 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 3 | 0.18 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 16 | 0.18 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 16 | 0.18 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG21 | 20 | 0.18 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG22 | 20 | 0.18 |
| (1,3407) | 1:56:A:ILE:H | 1:56:A:ILE:HG23 | 20 | 0.18 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 15 | 0.18 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 15 | 0.18 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 15 | 0.18 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 15 | 0.18 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 15 | 0.18 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 15 | 0.18 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 17 | 0.18 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 17 | 0.18 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG2 | 2 | 0.18 |
| (1,3327) | 1:105:A:SER:H | 1:102:A:ARG:HG3 | 2 | 0.18 |
| (1,3277) | 1:105:A:SER:H | 1:106:A:LEU:HG | 9 | 0.18 |
| (1,3264) | 1:147:A:ASN:H | 1:145:A:ARG:HG2 | 1 | 0.18 |
| (1,3264) | 1:147:A:ASN:H | 1:145:A:ARG:HG2 | 1 | 0.18 |
| (1,3264) | 1:147:A:ASN:H | 1:145:A:ARG:HG3 | 1 | 0.18 |
| (1,3264) | 1:147:A:ASN:H | 1:145:A:ARG:HG3 | 1 | 0.18 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB2 | 20 | 0.18 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HB3 | 20 | 0.18 |
| (1,3214) | 1:57:A:LYS:H | 1:66:A:VAL:HB | 8 | 0.18 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 2 | 0.18 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 15 | 0.18 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 17 | 0.18 |
| (1,3116) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 10 | 0.18 |
| (1,3116) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 10 | 0.18 |
| (1,3116) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 10 | 0.18 |
| (1,2324) | 1:49:A:VAL:HB | 1:50:A:GLU:H | 7 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 1 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 18 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 18 | 0.18 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 18 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 4 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 11 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 19 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 2 | 0.18 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 2 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 7 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 11 | 0.18 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG2 | 19 | 0.18 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG3 | 19 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 10 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 14 | 0.18 |
| (1,1745) | 1:50:A:GLU:H | 1:49:A:VAL:HB | 7 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD11 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD11 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD12 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD12 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD13 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD13 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD21 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD21 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD22 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD22 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD23 | 17 | 0.18 |
| (1,1658) | 1:106:A:LEU:HB3 | 1:108:A:LEU:HD23 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 19 | 0.18 |
| (1,1382) | 1:27:A:ALA:HB2 | 1:26:A:GLU:HB2 | 4 | 0.18 |
| (1,1382) | 1:27:A:ALA:HB2 | 1:26:A:GLU:HB3 | 4 | 0.18 |
| (1,1331) | 1:12:A:VAL:HG23 | 1:31:A:THR:HB | 7 | 0.18 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 9 | 0.18 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 9 | 0.18 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 9 | 0.18 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 9 | 0.18 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD2 | 18 | 0.18 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD3 | 18 | 0.18 |
| (1,59) | 1:93:A:PHE:HD2 | 1:91:A:VAL:HB | 12 | 0.18 |
| (1,3671) | 1:65:A:ILE:HG12 | 1:66:A:VAL:H | 20 | 0.17 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 6 | 0.17 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 2 | 0.17 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 2 | 0.17 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG2 | 1 | 0.17 |
| (1,3585) | 1:84:A:THR:H | 1:50:A:GLU:HG3 | 1 | 0.17 |
| (1,3585) | 1:84:A:THR:H | 1:38:A:VAL:HB | 13 | 0.17 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 17 | 0.17 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 17 | 0.17 |
| (1,3515) | 1:87:A:SER:H | 1:37:A:LYS:H | 17 | 0.17 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 8 | 0.17 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 8 | 0.17 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 10 | 0.17 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 10 | 0.17 |
| (1,3477) | 1:37:A:LYS:H | 1:87:A:SER:H | 17 | 0.17 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 1 | 0.17 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 1 | 0.17 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 1 | 0.17 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 9 | 0.17 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 9 | 0.17 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 9 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 2 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 2 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 10 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 14 | 0.17 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 14 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 1 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 1 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 1 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 4 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 4 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 4 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 13 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 13 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 13 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 14 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 14 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 14 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 16 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 16 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 16 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 18 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 18 | 0.17 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 18 | 0.17 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG2 | 2 | 0.17 |
| (1,3332) | 1:13:A:GLY:H | 1:30:A:LYS:HG3 | 2 | 0.17 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB2 | 4 | 0.17 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB3 | 4 | 0.17 |
| (1,3277) | 1:105:A:SER:H | 1:106:A:LEU:HG | 3 | 0.17 |
| (1,3277) | 1:105:A:SER:H | 1:106:A:LEU:HG | 15 | 0.17 |
| (1,3262) | 1:40:A:VAL:H | 1:50:A:GLU:HB2 | 15 | 0.17 |
| (1,3262) | 1:40:A:VAL:H | 1:50:A:GLU:HB3 | 15 | 0.17 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HG2 | 5 | 0.17 |
| (1,3236) | 1:75:A:TYR:H | 1:67:A:GLU:HG3 | 5 | 0.17 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 16 | 0.17 |
| (1,1947) | 1:91:A:VAL:HG12 | 1:30:A:LYS:HB2 | 14 | 0.17 |
| (1,1947) | 1:91:A:VAL:HG12 | 1:30:A:LYS:HB3 | 14 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 12 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 7 | 0.17 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 7 | 0.17 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 20 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 2 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 5 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 8 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 8 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 17 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 9 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 9 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 9 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 9 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 9 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 9 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 9 | 0.17 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 9 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 17 | 0.17 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 17 | 0.17 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 15 | 0.17 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:29:A:ILE:HA | 4 | 0.17 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:31:A:THR:HB | 17 | 0.17 |
| (1,770) | 1:60:A:LEU:HG | 1:59:A:PRO:HA | 15 | 0.17 |
| (1,3654) | 1:36:A:VAL:HB | 1:53:A:ASP:H | 18 | 0.16 |
| (1,3640) | 1:81:A:ASN:HB2 | 1:41:A:THR:H | 6 | 0.16 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG2 | 17 | 0.16 |
| (1,3591) | 1:89:A:TYR:H | 1:102:A:ARG:HG3 | 17 | 0.16 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 7 | 0.16 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 7 | 0.16 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG11 | 11 | 0.16 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG12 | 11 | 0.16 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG13 | 11 | 0.16 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG21 | 11 | 0.16 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG22 | 11 | 0.16 |
| (1,3406) | 1:55:A:HIS:H | 1:51:A:VAL:HG23 | 11 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG11 | 5 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG12 | 5 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG13 | 5 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG21 | 5 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG22 | 5 | 0.16 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG23 | 5 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 4 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 4 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 4 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 6 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 6 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 6 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 8 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 8 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 8 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 13 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 13 | 0.16 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 13 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 19 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 19 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 19 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 19 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 19 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 19 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 20 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 20 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 20 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 20 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 20 | 0.16 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 20 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 6 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 6 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 6 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 8 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 8 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 8 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 15 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 15 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 15 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 20 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 20 | 0.16 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 20 | 0.16 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD11 | 8 | 0.16 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD12 | 8 | 0.16 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD13 | 8 | 0.16 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD21 | 8 | 0.16 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD22 | 8 | 0.16 |
| (1,3341) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HD23 | 8 | 0.16 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG2 | 19 | 0.16 |
| (1,3294) | 1:34:A:ARG:H | 1:33:A:LYS:HG3 | 19 | 0.16 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD2 | 20 | 0.16 |
| (1,3288) | 1:57:A:LYS:H | 1:57:A:LYS:HD3 | 20 | 0.16 |
| (1,3214) | 1:57:A:LYS:H | 1:66:A:VAL:HB | 19 | 0.16 |
| (1,2421) | 1:37:A:LYS:HB2 | 1:38:A:VAL:H | 13 | 0.16 |
| (1,2421) | 1:37:A:LYS:HB3 | 1:38:A:VAL:H | 13 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 2 | 0.16 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 2 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 11 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 15 | 0.16 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB1 | 16 | 0.16 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB2 | 16 | 0.16 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB3 | 16 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 4 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 1 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 8 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 11 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 11 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 7 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB2 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB2 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB2 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB2 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD2 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB2 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB2 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB2 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB3 | 19 | 0.16 |
| (1,1842) | 1:43:A:ARG:HD3 | 1:43:A:ARG:HB3 | 19 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG13 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG13 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG13 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG13 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB2 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG13 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG13 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG11 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG12 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG13 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG13 | 16 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG21 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG22 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1816) | 1:53:A:ASP:HB3 | 1:36:A:VAL:HG23 | 16 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 4 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 5 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 6 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 6 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 7 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 12 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 12 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 14 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 9 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 10 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 19 | 0.16 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG2 | 5 | 0.16 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG3 | 5 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 6 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 6 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 8 | 0.16 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 8 | 0.16 |
| (1,1419) | 1:100:A:THR:HG23 | 1:89:A:TYR:H | 1 | 0.16 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD1 | 20 | 0.16 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD2 | 20 | 0.16 |
| (1,326) | 1:25:A:CYS:HA | 1:26:A:GLU:HG2 | 14 | 0.16 |
| (1,326) | 1:25:A:CYS:HA | 1:26:A:GLU:HG3 | 14 | 0.16 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB1 | 3 | 0.15 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB2 | 3 | 0.15 |
| (1,3596) | 1:106:A:LEU:H | 1:18:A:ALA:HB3 | 3 | 0.15 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 2 | 0.15 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 2 | 0.15 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 4 | 0.15 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 4 | 0.15 |
| (1,3493) | 1:69:A:LYS:H | 1:42:A:PHE:HE1 | 9 | 0.15 |
| (1,3493) | 1:69:A:LYS:H | 1:42:A:PHE:HE2 | 9 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 19 | 0.15 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 19 | 0.15 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 19 | 0.15 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 19 | 0.15 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 19 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 20 | 0.15 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 20 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 20 | 0.15 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 3 | 0.15 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 3 | 0.15 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 3 | 0.15 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 10 | 0.15 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 10 | 0.15 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 10 | 0.15 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB2 | 15 | 0.15 |
| (1,3306) | 1:90:A:THR:H | 1:30:A:LYS:HB3 | 15 | 0.15 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HG | 10 | 0.15 |
| (1,3217) | 1:38:A:VAL:H | 1:38:A:VAL:HB | 12 | 0.15 |
| (1,3151) | 1:80:A:ILE:H | 1:81:A:ASN:HA | 12 | 0.15 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 4 | 0.15 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 8 | 0.15 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 9 | 0.15 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 15 | 0.15 |
| (1,2618) | 1:9:A:TYR:HB2 | 1:10:A:LEU:H | 4 | 0.15 |
| (1,2618) | 1:9:A:TYR:HB3 | 1:10:A:LEU:H | 4 | 0.15 |
| (1,2319) | 1:67:A:GLU:HB2 | 1:68:A:VAL:H | 1 | 0.15 |
| (1,2319) | 1:67:A:GLU:HB3 | 1:68:A:VAL:H | 1 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 6 | 0.15 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB2 | 1 | 0.15 |
| (1,1947) | 1:91:A:VAL:HG13 | 1:30:A:LYS:HB3 | 1 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE2 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB2 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1946) | 1:39:A:LYS:HE3 | 1:39:A:LYS:HB3 | 18 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 1 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 2 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 3 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 7 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 8 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 10 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 13 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 13 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 14 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 16 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 17 | 0.15 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 17 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 19 | 0.15 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 14 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 20 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 3 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 4 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 6 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 12 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 14 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 15 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 17 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 19 | 0.15 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 19 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 20 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 17 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 3 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 14 | 0.15 |
| (1,1827) | 1:65:A:ILE:HA | 1:79:A:VAL:HB | 5 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 8 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 16 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 1 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 6 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 8 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 9 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 16 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 16 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB1 | 1:35:A:LEU:HB2 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB1 | 1:35:A:LEU:HB2 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB1 | 1:35:A:LEU:HB3 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB1 | 1:35:A:LEU:HB3 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB2 | 1:35:A:LEU:HB2 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB2 | 1:35:A:LEU:HB2 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB2 | 1:35:A:LEU:HB3 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB2 | 1:35:A:LEU:HB3 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB3 | 1:35:A:LEU:HB2 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB3 | 1:35:A:LEU:HB2 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB3 | 1:35:A:LEU:HB3 | 14 | 0.15 |
| (1,1612) | 1:86:A:ALA:HB3 | 1:35:A:LEU:HB3 | 14 | 0.15 |
| (1,1500) | 1:56:A:ILE:HD11 | 1:55:A:HIS:HA | 1 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 12 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 18 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 18 | 0.15 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 18 | 0.15 |
| (1,1402) | 1:29:A:ILE:HD13 | 1:17:A:SER:H | 19 | 0.15 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD1 | 2 | 0.15 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD2 | 2 | 0.15 |
| (1,1341) | 1:16:A:VAL:HG22 | 1:89:A:TYR:HB2 | 11 | 0.15 |
| (1,1341) | 1:16:A:VAL:HG22 | 1:89:A:TYR:HB3 | 11 | 0.15 |
| (1,1341) | 1:16:A:VAL:HG13 | 1:89:A:TYR:HB2 | 19 | 0.15 |
| (1,1341) | 1:16:A:VAL:HG13 | 1:89:A:TYR:HB3 | 19 | 0.15 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 1 | 0.15 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 3 | 0.15 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 12 | 0.15 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE2 | 6 | 0.15 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE3 | 6 | 0.15 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE2 | 6 | 0.15 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE3 | 6 | 0.15 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE2 | 6 | 0.15 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE3 | 6 | 0.15 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 7 | 0.15 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 7 | 0.15 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 7 | 0.15 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 7 | 0.15 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 19 | 0.15 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 19 | 0.15 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 19 | 0.15 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD2 | 7 | 0.15 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD3 | 7 | 0.15 |
| (1,3714) | 1:115:A:ALA:HB3 | 1:114:A:PHE:H | 19 | 0.14 |
| (1,3654) | 1:36:A:VAL:HB | 1:53:A:ASP:H | 12 | 0.14 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 15 | 0.14 |
| (1,3599) | 1:76:A:GLN:HE21 | 1:76:A:GLN:HA | 9 | 0.14 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 9 | 0.14 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 9 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 1 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 1 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 1 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 1 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 1 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 1 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD11 | 15 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD12 | 15 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD13 | 15 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD21 | 15 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD22 | 15 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:106:A:LEU:HD23 | 15 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG11 | 17 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG12 | 17 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG13 | 17 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG21 | 17 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG22 | 17 | 0.14 |
| (1,3399) | 1:107:A:CYS:H | 1:16:A:VAL:HG23 | 17 | 0.14 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 11 | 0.14 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 11 | 0.14 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 11 | 0.14 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG21 | 20 | 0.14 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG22 | 20 | 0.14 |
| (1,3367) | 1:14:A:THR:H | 1:14:A:THR:HG23 | 20 | 0.14 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 10 | 0.14 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 10 | 0.14 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 10 | 0.14 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 10 | 0.14 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 10 | 0.14 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 10 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 13 | 0.14 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 13 | 0.14 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 11 | 0.14 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 11 | 0.14 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 11 | 0.14 |
| (1,3299) | 1:108:A:LEU:H | 1:109:A:LYS:HG2 | 7 | 0.14 |
| (1,3299) | 1:108:A:LEU:H | 1:109:A:LYS:HG3 | 7 | 0.14 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 4 | 0.14 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 7 | 0.14 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 9 | 0.14 |
| (1,2618) | 1:9:A:TYR:HB2 | 1:10:A:LEU:H | 18 | 0.14 |
| (1,2618) | 1:9:A:TYR:HB3 | 1:10:A:LEU:H | 18 | 0.14 |
| (1,2469) | 1:101:A:LEU:HD11 | 1:101:A:LEU:H | 20 | 0.14 |
| (1,2469) | 1:101:A:LEU:HD12 | 1:101:A:LEU:H | 20 | 0.14 |
| (1,2469) | 1:101:A:LEU:HD13 | 1:101:A:LEU:H | 20 | 0.14 |
| (1,2469) | 1:101:A:LEU:HD21 | 1:101:A:LEU:H | 20 | 0.14 |
| (1,2469) | 1:101:A:LEU:HD22 | 1:101:A:LEU:H | 20 | 0.14 |
| (1,2469) | 1:101:A:LEU:HD23 | 1:101:A:LEU:H | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 5 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 20 | 0.14 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 1 | 0.14 |
| (1,1851) | 1:11:A:THR:HA | 1:14:A:THR:HB | 3 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 5 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 7 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 9 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG2 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB2 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1844) | 1:43:A:ARG:HG3 | 1:43:A:ARG:HB3 | 13 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 11 | 0.14 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 11 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 17 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG2 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD2 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1805) | 1:34:A:ARG:HG3 | 1:34:A:ARG:HD3 | 18 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 14 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 14 | 0.14 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 14 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 4 | 0.14 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1768) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 4 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 5 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 7 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 13 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 19 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG2 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD2 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1767) | 1:21:A:ARG:HG3 | 1:21:A:ARG:HD3 | 20 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 11 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 1 | 0.14 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 1 | 0.14 |
| (1,1629) | 1:91:A:VAL:HG21 | 1:93:A:PHE:HA | 4 | 0.14 |
| (1,1500) | 1:56:A:ILE:HD12 | 1:55:A:HIS:HA | 12 | 0.14 |
| (1,1500) | 1:56:A:ILE:HD13 | 1:55:A:HIS:HA | 18 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 3 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 3 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 16 | 0.14 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 16 | 0.14 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE2 | 3 | 0.14 |
| (1,1456) | 1:92:A:VAL:HB | 1:28:A:LYS:HE3 | 3 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1405) | 1:29:A:ILE:HD13 | 1:32:A:ALA:HA | 3 | 0.14 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:12:A:VAL:H | 8 | 0.14 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD1 | 1 | 0.14 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD2 | 1 | 0.14 |
| (1,1315) | 1:115:A:ALA:HA | 1:114:A:PHE:H | 8 | 0.14 |
| (1,1055) | 1:106:A:LEU:HD11 | 1:90:A:THR:HA | 8 | 0.14 |
| (1,1055) | 1:106:A:LEU:HD12 | 1:90:A:THR:HA | 8 | 0.14 |
| (1,1055) | 1:106:A:LEU:HD13 | 1:90:A:THR:HA | 8 | 0.14 |
| (1,1055) | 1:106:A:LEU:HD21 | 1:90:A:THR:HA | 8 | 0.14 |
| (1,1055) | 1:106:A:LEU:HD22 | 1:90:A:THR:HA | 8 | 0.14 |
| (1,1055) | 1:106:A:LEU:HD23 | 1:90:A:THR:HA | 8 | 0.14 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 13 | 0.14 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 13 | 0.14 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 13 | 0.14 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 19 | 0.14 |
| (1,72) | 1:75:A:TYR:HE2 | 1:75:A:TYR:HA | 7 | 0.14 |
| (1,2) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD1 | 12 | 0.14 |
| (1,2) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD2 | 12 | 0.14 |
| (1,2) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD1 | 12 | 0.14 |
| (1,2) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD2 | 12 | 0.14 |
| (1,1) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD1 | 12 | 0.14 |
| (1,1) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD2 | 12 | 0.14 |
| (1,1) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD1 | 12 | 0.14 |
| (1,1) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD2 | 12 | 0.14 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB2 | 20 | 0.13 |
| (1,3529) | 1:88:A:TRP:HE1 | 1:101:A:LEU:HB3 | 20 | 0.13 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 13 | 0.13 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 13 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG11 | 4 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG12 | 4 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG13 | 4 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG21 | 4 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG22 | 4 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG23 | 4 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG11 | 14 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG12 | 14 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG13 | 14 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG21 | 14 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG22 | 14 | 0.13 |
| (1,3387) | 1:61:A:LYS:H | 1:66:A:VAL:HG23 | 14 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG11 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG12 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG13 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG21 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG22 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 3 | 0.13 |
| (1,3378) | 1:38:A:VAL:H | 1:38:A:VAL:HG23 | 3 | 0.13 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 17 | 0.13 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 17 | 0.13 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 17 | 0.13 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 17 | 0.13 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 17 | 0.13 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 17 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 2 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 2 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 2 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 9 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 9 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 9 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 19 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 19 | 0.13 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 19 | 0.13 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 1 | 0.13 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 1 | 0.13 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG2 | 5 | 0.13 |
| (1,3310) | 1:49:A:VAL:H | 1:39:A:LYS:HG3 | 5 | 0.13 |
| (1,3271) | 1:60:A:LEU:H | 1:60:A:LEU:HB2 | 6 | 0.13 |
| (1,3271) | 1:60:A:LEU:H | 1:60:A:LEU:HB3 | 6 | 0.13 |
| (1,3258) | 1:109:A:LYS:H | 1:109:A:LYS:HB2 | 14 | 0.13 |
| (1,3258) | 1:109:A:LYS:H | 1:109:A:LYS:HB3 | 14 | 0.13 |
| (1,3217) | 1:38:A:VAL:H | 1:38:A:VAL:HB | 19 | 0.13 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 12 | 0.13 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 5 | 0.13 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 13 | 0.13 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 15 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 9 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 9 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 9 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 9 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 9 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 15 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 15 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 15 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 15 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 15 | 0.13 |
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 15 | 0.13 |
| (1,2464) | 1:10:A:LEU:HG | 1:11:A:THR:H | 17 | 0.13 |
| (1,2447) | 1:99:A:LYS:HG2 | 1:98:A:GLU:H | 18 | 0.13 |
| (1,2447) | 1:99:A:LYS:HG3 | 1:98:A:GLU:H | 18 | 0.13 |
| (1,1976) | 1:110:A:GLY:HA2 | 1:108:A:LEU:HB2 | 7 | 0.13 |
| (1,1976) | 1:110:A:GLY:HA2 | 1:108:A:LEU:HB3 | 7 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 13 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB2 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG2 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB2 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1932) | 1:99:A:LYS:HG3 | 1:99:A:LYS:HB3 | 4 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG11 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG12 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG13 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1872) | 1:38:A:VAL:HG21 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG22 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG12 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1872) | 1:38:A:VAL:HG23 | 1:56:A:ILE:HG13 | 14 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 20 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB2 | 1:39:A:LYS:HE2 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB2 | 1:39:A:LYS:HE2 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB2 | 1:39:A:LYS:HE2 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB2 | 1:39:A:LYS:HE3 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB2 | 1:39:A:LYS:HE3 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB2 | 1:39:A:LYS:HE3 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB3 | 1:39:A:LYS:HE2 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB3 | 1:39:A:LYS:HE2 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB3 | 1:39:A:LYS:HE2 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1835) | 1:82:A:LYS:HB3 | 1:39:A:LYS:HE3 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB3 | 1:39:A:LYS:HE3 | 2 | 0.13 |
| (1,1835) | 1:82:A:LYS:HB3 | 1:39:A:LYS:HE3 | 2 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB2 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE2 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB2 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1800) | 1:33:A:LYS:HE3 | 1:33:A:LYS:HB3 | 15 | 0.13 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG2 | 2 | 0.13 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG3 | 2 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG11 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG12 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG13 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG21 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG22 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB2 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1775) | 1:92:A:VAL:HG23 | 1:28:A:LYS:HB3 | 9 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB2 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB2 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1772) | 1:20:A:TYR:HB3 | 1:25:A:CYS:HB3 | 7 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 13 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 16 | 0.13 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 16 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD11 | 1:43:A:ARG:HD2 | 6 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1540) | 1:65:A:ILE:HD11 | 1:43:A:ARG:HD2 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD11 | 1:43:A:ARG:HD3 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD11 | 1:43:A:ARG:HD3 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD12 | 1:43:A:ARG:HD2 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD12 | 1:43:A:ARG:HD2 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD12 | 1:43:A:ARG:HD3 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD12 | 1:43:A:ARG:HD3 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD13 | 1:43:A:ARG:HD2 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD13 | 1:43:A:ARG:HD2 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD13 | 1:43:A:ARG:HD3 | 6 | 0.13 |
| (1,1540) | 1:65:A:ILE:HD13 | 1:43:A:ARG:HD3 | 6 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG11 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG12 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG13 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG21 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG22 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG12 | 1:38:A:VAL:HG23 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG11 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG12 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG13 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG21 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG22 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 2 | 0.13 |
| (1,1496) | 1:56:A:ILE:HG13 | 1:38:A:VAL:HG23 | 2 | 0.13 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG11 | 11 | 0.13 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG12 | 11 | 0.13 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG13 | 11 | 0.13 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG21 | 11 | 0.13 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG22 | 11 | 0.13 |
| (1,1484) | 1:50:A:GLU:HA | 1:49:A:VAL:HG23 | 11 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 13 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 17 | 0.13 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 17 | 0.13 |
| (1,1431) | 1:35:A:LEU:HG | 1:36:A:VAL:H | 6 | 0.13 |
| (1,1405) | 1:29:A:ILE:HD13 | 1:32:A:ALA:HA | 6 | 0.13 |
| (1,1402) | 1:29:A:ILE:HD11 | 1:17:A:SER:H | 1 | 0.13 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 11 | 0.13 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 18 | 0.13 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 19 | 0.13 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 4 | 0.13 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 4 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 4 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 4 | 0.13 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 6 | 0.13 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 6 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 6 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 6 | 0.13 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 12 | 0.13 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 12 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 12 | 0.13 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 12 | 0.13 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 10 | 0.13 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD2 | 16 | 0.13 |
| (1,357) | 1:34:A:ARG:HA | 1:33:A:LYS:HD3 | 16 | 0.13 |
| (2,73) | 1:109:A:LYS:H | 1:15:A:ASP:O | 9 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 3 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 6 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 18 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 18 | 0.12 |
| (1,3654) | 1:36:A:VAL:HB | 1:53:A:ASP:H | 6 | 0.12 |
| (1,3654) | 1:36:A:VAL:HB | 1:53:A:ASP:H | 19 | 0.12 |
| (1,3640) | 1:81:A:ASN:HB2 | 1:41:A:THR:H | 3 | 0.12 |
| (1,3596) | 1:106:A:LEU:H | 1:102:A:ARG:HG2 | 14 | 0.12 |
| (1,3596) | 1:106:A:LEU:H | 1:102:A:ARG:HG3 | 14 | 0.12 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 7 | 0.12 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 7 | 0.12 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB2 | 15 | 0.12 |
| (1,3579) | 1:76:A:GLN:H | 1:69:A:LYS:HB3 | 15 | 0.12 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB2 | 11 | 0.12 |
| (1,3541) | 1:38:A:VAL:H | 1:53:A:ASP:HB3 | 11 | 0.12 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 14 | 0.12 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 14 | 0.12 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 16 | 0.12 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 16 | 0.12 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 16 | 0.12 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 16 | 0.12 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 16 | 0.12 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 16 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD11 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD12 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD13 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD21 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD22 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 6 | 0.12 |
| (1,3356) | 1:71:A:LEU:H | 1:71:A:LEU:HD23 | 6 | 0.12 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 5 | 0.12 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 5 | 0.12 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 17 | 0.12 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 17 | 0.12 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 17 | 0.12 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB2 | 3 | 0.12 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB3 | 3 | 0.12 |
| (1,3214) | 1:57:A:LYS:H | 1:66:A:VAL:HB | 1 | 0.12 |
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 6 | 0.12 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 7 | 0.12 |
| (1,2481) | 1:80:A:ILE:HD11 | 1:80:A:ILE:H | 8 | 0.12 |
| (1,2481) | 1:80:A:ILE:HD12 | 1:80:A:ILE:H | 8 | 0.12 |
| (1,2481) | 1:80:A:ILE:HD13 | 1:80:A:ILE:H | 8 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 4 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 4 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 4 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 4 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 4 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 4 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 8 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 8 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 8 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 8 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 8 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 8 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 12 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 12 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 12 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 12 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 12 | 0.12 |
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 12 | 0.12 |
| (1,2464) | 1:10:A:LEU:HG | 1:11:A:THR:H | 15 | 0.12 |
| (1,2447) | 1:99:A:LYS:HG2 | 1:98:A:GLU:H | 12 | 0.12 |
| (1,2447) | 1:99:A:LYS:HG3 | 1:98:A:GLU:H | 12 | 0.12 |
| (1,2358) | 1:52:A:GLN:HB2 | 1:52:A:GLN:HE21 | 3 | 0.12 |
| (1,2358) | 1:52:A:GLN:HB2 | 1:52:A:GLN:HE22 | 3 | 0.12 |
| (1,2358) | 1:52:A:GLN:HB3 | 1:52:A:GLN:HE21 | 3 | 0.12 |
| (1,2358) | 1:52:A:GLN:HB3 | 1:52:A:GLN:HE22 | 3 | 0.12 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB1 | 10 | 0.12 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB2 | 10 | 0.12 |
| (1,1891) | 1:68:A:VAL:HB | 1:78:A:ALA:HB3 | 10 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 18 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD2 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB2 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD2 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1849) | 1:142:A:ARG:HB3 | 1:142:A:ARG:HD3 | 18 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD2 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB2 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1843) | 1:145:A:ARG:HD3 | 1:145:A:ARG:HB3 | 11 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 20 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB2 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB2 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1752) | 1:24:A:PHE:HB3 | 1:17:A:SER:HB3 | 5 | 0.12 |
| (1,1644) | 1:101:A:LEU:HD11 | 1:99:A:LYS:HA | 14 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 8 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 9 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 17 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 19 | 0.12 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 19 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 2 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 3 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 5 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 6 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 10 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 11 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 13 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 13 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 14 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 16 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 18 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 20 | 0.12 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 20 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 9 | 0.12 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 9 | 0.12 |
| (1,1431) | 1:35:A:LEU:HG | 1:36:A:VAL:H | 4 | 0.12 |
| (1,1431) | 1:35:A:LEU:HG | 1:36:A:VAL:H | 12 | 0.12 |
| (1,1402) | 1:29:A:ILE:HD12 | 1:17:A:SER:H | 18 | 0.12 |
| (1,1401) | 1:29:A:ILE:HD12 | 1:16:A:VAL:H | 10 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE2 | 14 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE3 | 14 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE2 | 14 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE3 | 14 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE2 | 14 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE3 | 14 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE2 | 16 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB1 | 1:33:A:LYS:HE3 | 16 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE2 | 16 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB2 | 1:33:A:LYS:HE3 | 16 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE2 | 16 | 0.12 |
| (1,1121) | 1:32:A:ALA:HB3 | 1:33:A:LYS:HE3 | 16 | 0.12 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 8 | 0.12 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 8 | 0.12 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 8 | 0.12 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 8 | 0.12 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB2 | 15 | 0.12 |
| (1,871) | 1:70:A:ASN:HD21 | 1:69:A:LYS:HB3 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB2 | 15 | 0.12 |
| (1,871) | 1:70:A:ASN:HD22 | 1:69:A:LYS:HB3 | 15 | 0.12 |
| (1,654) | 1:69:A:LYS:H | 1:51:A:VAL:HG11 | 2 | 0.12 |
| (1,654) | 1:69:A:LYS:H | 1:51:A:VAL:HG12 | 2 | 0.12 |
| (1,654) | 1:69:A:LYS:H | 1:51:A:VAL:HG13 | 2 | 0.12 |
| (1,654) | 1:69:A:LYS:H | 1:51:A:VAL:HG21 | 2 | 0.12 |
| (1,654) | 1:69:A:LYS:H | 1:51:A:VAL:HG22 | 2 | 0.12 |
| (1,654) | 1:69:A:LYS:H | 1:51:A:VAL:HG23 | 2 | 0.12 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 6 | 0.12 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 7 | 0.12 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG2 | 15 | 0.12 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG2 | 15 | 0.12 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG3 | 15 | 0.12 |
| (1,59) | 1:93:A:PHE:HD2 | 1:99:A:LYS:HG3 | 15 | 0.12 |
| (1,51) | 1:10:A:LEU:HB2 | 1:9:A:TYR:HD1 | 4 | 0.12 |
| (1,51) | 1:10:A:LEU:HB2 | 1:9:A:TYR:HD2 | 4 | 0.12 |
| (1,51) | 1:10:A:LEU:HB3 | 1:9:A:TYR:HD1 | 4 | 0.12 |
| (1,51) | 1:10:A:LEU:HB3 | 1:9:A:TYR:HD2 | 4 | 0.12 |
| (1,2) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD1 | 5 | 0.12 |
| (1,2) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD2 | 5 | 0.12 |
| (1,2) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD1 | 5 | 0.12 |
| (1,2) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD2 | 5 | 0.12 |
| (1,1) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD1 | 5 | 0.12 |
| (1,1) | 1:8:A:PRO:HB2 | 1:9:A:TYR:HD2 | 5 | 0.12 |
| (1,1) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD1 | 5 | 0.12 |
| (1,1) | 1:8:A:PRO:HB3 | 1:9:A:TYR:HD2 | 5 | 0.12 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 13 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 20 | 0.11 |
| (1,3654) | 1:36:A:VAL:HB | 1:53:A:ASP:H | 5 | 0.11 |
| (1,3654) | 1:36:A:VAL:HB | 1:53:A:ASP:H | 10 | 0.11 |
| (1,3610) | 1:93:A:PHE:HA | 1:97:A:ASP:H | 20 | 0.11 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG2 | 11 | 0.11 |
| (1,3601) | 1:81:A:ASN:H | 1:39:A:LYS:HG3 | 11 | 0.11 |
| (1,3599) | 1:76:A:GLN:HE21 | 1:76:A:GLN:HA | 19 | 0.11 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 6 | 0.11 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 6 | 0.11 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 12 | 0.11 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 12 | 0.11 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 15 | 0.11 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 15 | 0.11 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 5 | 0.11 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 5 | 0.11 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 5 | 0.11 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 5 | 0.11 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 5 | 0.11 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 5 | 0.11 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG21 | 7 | 0.11 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG22 | 7 | 0.11 |
| (1,3351) | 1:90:A:THR:H | 1:90:A:THR:HG23 | 7 | 0.11 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD2 | 8 | 0.11 |
| (1,3325) | 1:67:A:GLU:H | 1:57:A:LYS:HD3 | 8 | 0.11 |
| (1,3293) | 1:36:A:VAL:H | 1:35:A:LEU:HG | 9 | 0.11 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB2 | 1 | 0.11 |
| (1,3280) | 1:9:A:TYR:H | 1:108:A:LEU:HB3 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3134) | 1:57:A:LYS:H | 1:68:A:VAL:HA | 10 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 2 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 2 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 2 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 15 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 15 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 15 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 16 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 16 | 0.11 |
| (1,3116) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 16 | 0.11 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 3 | 0.11 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 19 | 0.11 |
| (1,2618) | 1:9:A:TYR:HB2 | 1:10:A:LEU:H | 10 | 0.11 |
| (1,2618) | 1:9:A:TYR:HB3 | 1:10:A:LEU:H | 10 | 0.11 |
| (1,2615) | 1:87:A:SER:HB2 | 1:33:A:LYS:H | 4 | 0.11 |
| (1,2615) | 1:87:A:SER:HB3 | 1:33:A:LYS:H | 4 | 0.11 |
| (1,2481) | 1:80:A:ILE:HD11 | 1:80:A:ILE:H | 17 | 0.11 |
| (1,2481) | 1:80:A:ILE:HD12 | 1:80:A:ILE:H | 17 | 0.11 |
| (1,2481) | 1:80:A:ILE:HD13 | 1:80:A:ILE:H | 17 | 0.11 |
| (1,2477) | 1:86:A:ALA:HB1 | 1:37:A:LYS:H | 16 | 0.11 |
| (1,2477) | 1:86:A:ALA:HB2 | 1:37:A:LYS:H | 16 | 0.11 |
| (1,2477) | 1:86:A:ALA:HB3 | 1:37:A:LYS:H | 16 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD2 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB2 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1972) | 1:112:A:ARG:HD3 | 1:112:A:ARG:HB3 | 1 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 11 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB2 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB2 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1967) | 1:17:A:SER:HB3 | 1:107:A:CYS:HB3 | 14 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE2 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG2 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1830) | 1:57:A:LYS:HE3 | 1:57:A:LYS:HG3 | 15 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE2 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG2 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1783) | 1:138:A:LYS:HE3 | 1:138:A:LYS:HG3 | 3 | 0.11 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG2 | 18 | 0.11 |
| (1,1780) | 1:26:A:GLU:HA | 1:109:A:LYS:HG3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1766) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 7 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1765) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 18 | 0.11 |
| (1,1575) | 1:78:A:ALA:HA | 1:43:A:ARG:HG2 | 15 | 0.11 |
| (1,1575) | 1:78:A:ALA:HA | 1:43:A:ARG:HG2 | 15 | 0.11 |
| (1,1575) | 1:78:A:ALA:HA | 1:43:A:ARG:HG3 | 15 | 0.11 |
| (1,1575) | 1:78:A:ALA:HA | 1:43:A:ARG:HG3 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 1 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 2 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 3 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 4 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 5 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 6 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 7 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 10 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 11 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 12 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 12 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 13 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 14 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 15 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 18 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD11 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD12 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD13 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD21 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD22 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 20 | 0.11 |
| (1,1561) | 1:71:A:LEU:HG | 1:71:A:LEU:HD23 | 20 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 1 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 4 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 7 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 8 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 9 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 12 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 12 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 15 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 17 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG11 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG12 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG13 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG21 | 19 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG22 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 19 | 0.11 |
| (1,1457) | 1:79:A:VAL:HB | 1:79:A:VAL:HG23 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 1 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 4 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 5 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 6 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 7 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 10 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 11 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 12 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 14 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 16 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 18 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 19 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 20 | 0.11 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 20 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 2 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 3 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 5 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 6 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 7 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 8 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 10 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 11 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 12 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 13 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 14 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 15 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 16 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 17 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 19 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 19 | 0.11 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 19 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1431) | 1:35:A:LEU:HG | 1:36:A:VAL:H | 9 | 0.11 |
| (1,1431) | 1:35:A:LEU:HG | 1:36:A:VAL:H | 20 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 6 | 0.11 |
| (1,1402) | 1:29:A:ILE:HD12 | 1:17:A:SER:H | 3 | 0.11 |
| (1,1382) | 1:27:A:ALA:HB2 | 1:16:A:VAL:HB | 11 | 0.11 |
| (1,1368) | 1:78:A:ALA:HA | 1:43:A:ARG:HG2 | 15 | 0.11 |
| (1,1368) | 1:78:A:ALA:HA | 1:43:A:ARG:HG2 | 15 | 0.11 |
| (1,1368) | 1:78:A:ALA:HA | 1:43:A:ARG:HG3 | 15 | 0.11 |
| (1,1368) | 1:78:A:ALA:HA | 1:43:A:ARG:HG3 | 15 | 0.11 |
| (1,1367) | 1:78:A:ALA:HA | 1:43:A:ARG:HG2 | 15 | 0.11 |
| (1,1367) | 1:78:A:ALA:HA | 1:43:A:ARG:HG2 | 15 | 0.11 |
| (1,1367) | 1:78:A:ALA:HA | 1:43:A:ARG:HG3 | 15 | 0.11 |
| (1,1367) | 1:78:A:ALA:HA | 1:43:A:ARG:HG3 | 15 | 0.11 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 4 | 0.11 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 17 | 0.11 |
| (1,687) | 1:54:A:ASP:HB2 | 1:52:A:GLN:HG2 | 8 | 0.11 |
| (1,687) | 1:54:A:ASP:HB2 | 1:52:A:GLN:HG3 | 8 | 0.11 |
| (1,687) | 1:54:A:ASP:HB3 | 1:52:A:GLN:HG2 | 8 | 0.11 |
| (1,687) | 1:54:A:ASP:HB3 | 1:52:A:GLN:HG3 | 8 | 0.11 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 8 | 0.11 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 8 | 0.11 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 8 | 0.11 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 10 | 0.11 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 10 | 0.11 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 10 | 0.11 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 11 | 0.11 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 11 | 0.11 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 11 | 0.11 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 19 | 0.11 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 19 | 0.11 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 19 | 0.11 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 9 | 0.11 |
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG2 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG2 | 1 | 0.11 |
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG3 | 1 | 0.11 |
| (1,59) | 1:93:A:PHE:HD1 | 1:99:A:LYS:HG3 | 1 | 0.11 |
| (2,73) | 1:109:A:LYS:H | 1:15:A:ASP:O | 2 | 0.1 |
| (1,3702) | 1:33:A:LYS:HE3 | 1:32:A:ALA:H | 6 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 1 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB2 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD21 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3684) | 1:141:A:ASN:HB3 | 1:141:A:ASN:HD22 | 12 | 0.1 |
| (1,3542) | 1:85:A:ASP:H | 1:37:A:LYS:HB2 | 10 | 0.1 |
| (1,3542) | 1:85:A:ASP:H | 1:37:A:LYS:HB3 | 10 | 0.1 |
| (1,3542) | 1:85:A:ASP:H | 1:83:A:LEU:HB2 | 17 | 0.1 |
| (1,3542) | 1:85:A:ASP:H | 1:83:A:LEU:HB3 | 17 | 0.1 |
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE1 | 18 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3502) | 1:10:A:LEU:H | 1:89:A:TYR:HE2 | 18 | 0.1 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD11 | 4 | 0.1 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD12 | 4 | 0.1 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD13 | 4 | 0.1 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD21 | 4 | 0.1 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD22 | 4 | 0.1 |
| (1,3411) | 1:105:A:SER:H | 1:101:A:LEU:HD23 | 4 | 0.1 |
| (1,3368) | 1:48:A:THR:HG23 | 1:41:A:THR:H | 9 | 0.1 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG11 | 7 | 0.1 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG12 | 7 | 0.1 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG13 | 7 | 0.1 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG21 | 7 | 0.1 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG22 | 7 | 0.1 |
| (1,3359) | 1:55:A:HIS:H | 1:68:A:VAL:HG23 | 7 | 0.1 |
| (1,3277) | 1:105:A:SER:H | 1:106:A:LEU:HG | 6 | 0.1 |
| (1,3271) | 1:60:A:LEU:H | 1:60:A:LEU:HB2 | 9 | 0.1 |
| (1,3271) | 1:60:A:LEU:H | 1:60:A:LEU:HB3 | 9 | 0.1 |
| (1,3209) | 1:26:A:GLU:H | 1:26:A:GLU:HG2 | 1 | 0.1 |
| (1,3209) | 1:26:A:GLU:H | 1:26:A:GLU:HG2 | 1 | 0.1 |
| (1,3209) | 1:26:A:GLU:H | 1:26:A:GLU:HG3 | 1 | 0.1 |
| (1,3209) | 1:26:A:GLU:H | 1:26:A:GLU:HG3 | 1 | 0.1 |
| (1,3116) | 1:29:A:ILE:HD11 | 1:10:A:LEU:H | 17 | 0.1 |
| (1,3116) | 1:29:A:ILE:HD12 | 1:10:A:LEU:H | 17 | 0.1 |
| (1,3116) | 1:29:A:ILE:HD13 | 1:10:A:LEU:H | 17 | 0.1 |
| (1,3093) | 1:87:A:SER:HB2 | 1:88:A:TRP:H | 13 | 0.1 |
| (1,3093) | 1:87:A:SER:HB3 | 1:88:A:TRP:H | 13 | 0.1 |
| (1,3066) | 1:70:A:ASN:HA | 1:74:A:ALA:H | 6 | 0.1 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 18 | 0.1 |
| (1,2681) | 1:97:A:ASP:H | 1:94:A:ASP:H | 20 | 0.1 |
| (1,2618) | 1:9:A:TYR:HB2 | 1:10:A:LEU:H | 9 | 0.1 |
| (1,2618) | 1:9:A:TYR:HB3 | 1:10:A:LEU:H | 9 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD11 | 1:80:A:ILE:H | 1 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD12 | 1:80:A:ILE:H | 1 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD13 | 1:80:A:ILE:H | 1 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD11 | 1:80:A:ILE:H | 3 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD12 | 1:80:A:ILE:H | 3 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD13 | 1:80:A:ILE:H | 3 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD11 | 1:80:A:ILE:H | 12 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD12 | 1:80:A:ILE:H | 12 | 0.1 |
| (1,2481) | 1:80:A:ILE:HD13 | 1:80:A:ILE:H | 12 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 3 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 3 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 3 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 3 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 3 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 3 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD11 | 1:108:A:LEU:H | 14 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD12 | 1:108:A:LEU:H | 14 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD13 | 1:108:A:LEU:H | 14 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD21 | 1:108:A:LEU:H | 14 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD22 | 1:108:A:LEU:H | 14 | 0.1 |
| (1,2478) | 1:108:A:LEU:HD23 | 1:108:A:LEU:H | 14 | 0.1 |
| (1,2464) | 1:10:A:LEU:HG | 1:11:A:THR:H | 7 | 0.1 |
| (1,2464) | 1:10:A:LEU:HG | 1:11:A:THR:H | 14 | 0.1 |
| (1,2447) | 1:99:A:LYS:HG2 | 1:98:A:GLU:H | 15 | 0.1 |
| (1,2447) | 1:99:A:LYS:HG3 | 1:98:A:GLU:H | 15 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD2 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB2 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1926) | 1:43:A:ARG:HD3 | 1:77:A:GLU:HB3 | 14 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG11 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG11 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG12 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG12 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG13 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG13 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG21 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG21 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG22 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG22 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG23 | 17 | 0.1 |
| (1,1897) | 1:54:A:ASP:H | 1:36:A:VAL:HG23 | 17 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 2 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 9 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG11 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG12 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG13 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG21 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG22 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 15 | 0.1 |
| (1,1441) | 1:38:A:VAL:HB | 1:38:A:VAL:HG23 | 15 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 1 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 1 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 4 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 18 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG11 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG12 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG13 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG21 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG22 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 20 | 0.1 |
| (1,1435) | 1:36:A:VAL:HB | 1:36:A:VAL:HG23 | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1433) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD11 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD12 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD13 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD21 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB2 | 14 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD22 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB2 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1429) | 1:35:A:LEU:HD23 | 1:35:A:LEU:HB3 | 14 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB1 | 1:89:A:TYR:HD1 | 17 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB1 | 1:89:A:TYR:HD2 | 17 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB2 | 1:89:A:TYR:HD1 | 18 | 0.1 |
| (1,1376) | 1:32:A:ALA:HB2 | 1:89:A:TYR:HD2 | 18 | 0.1 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD1 | 10 | 0.1 |
| (1,1361) | 1:21:A:ARG:HA | 1:20:A:TYR:HD2 | 10 | 0.1 |
| (1,1331) | 1:12:A:VAL:HG22 | 1:31:A:THR:HB | 6 | 0.1 |
| (1,1314) | 1:64:A:ALA:HA | 1:80:A:ILE:HB | 14 | 0.1 |
| (1,1119) | 1:86:A:ALA:HB1 | 1:37:A:LYS:HE2 | 7 | 0.1 |
| (1,1119) | 1:86:A:ALA:HB1 | 1:37:A:LYS:HE3 | 7 | 0.1 |
| (1,1119) | 1:86:A:ALA:HB2 | 1:37:A:LYS:HE2 | 7 | 0.1 |
| (1,1119) | 1:86:A:ALA:HB2 | 1:37:A:LYS:HE3 | 7 | 0.1 |
| (1,1119) | 1:86:A:ALA:HB3 | 1:37:A:LYS:HE2 | 7 | 0.1 |
| (1,1119) | 1:86:A:ALA:HB3 | 1:37:A:LYS:HE3 | 7 | 0.1 |
| (1,762) | 1:69:A:LYS:HE2 | 1:57:A:LYS:HD2 | 7 | 0.1 |
| (1,762) | 1:69:A:LYS:HE2 | 1:57:A:LYS:HD3 | 7 | 0.1 |
| (1,762) | 1:69:A:LYS:HE3 | 1:57:A:LYS:HD2 | 7 | 0.1 |
| (1,762) | 1:69:A:LYS:HE3 | 1:57:A:LYS:HD3 | 7 | 0.1 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 16 | 0.1 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 16 | 0.1 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 16 | 0.1 |
| (1,581) | 1:78:A:ALA:HB1 | 1:43:A:ARG:HA | 20 | 0.1 |
| (1,581) | 1:78:A:ALA:HB2 | 1:43:A:ARG:HA | 20 | 0.1 |
| (1,581) | 1:78:A:ALA:HB3 | 1:43:A:ARG:HA | 20 | 0.1 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 8 | 0.1 |
| (1,421) | 1:89:A:TYR:HA | 1:100:A:THR:HB | 20 | 0.1 |

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

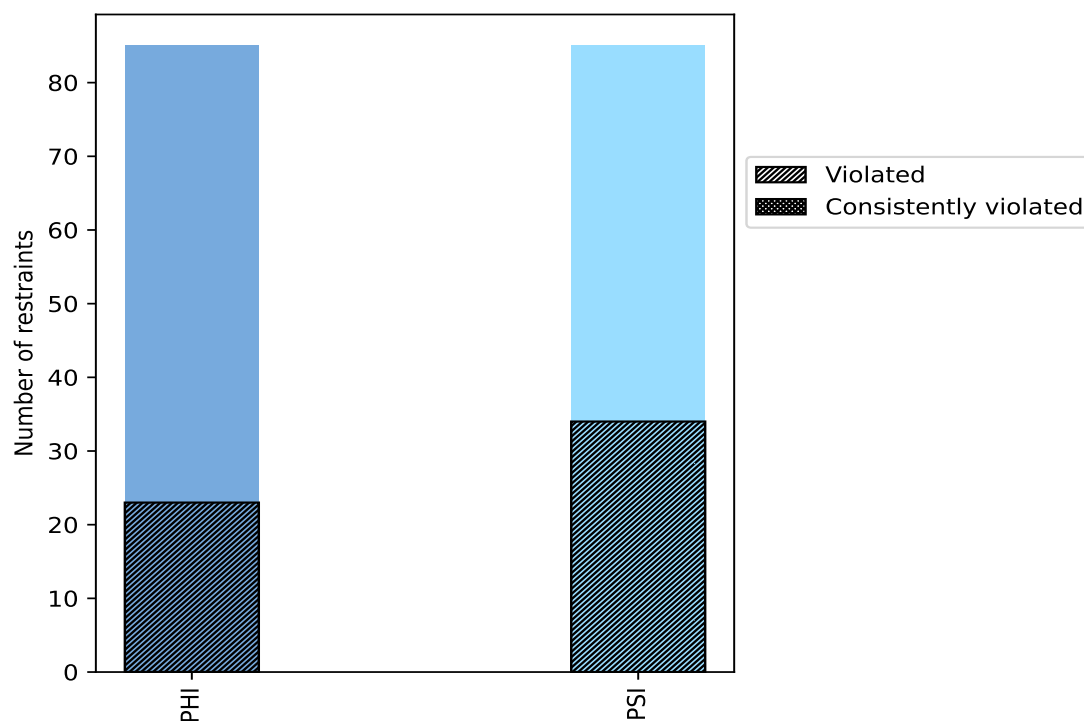
10.1 Summary of dihedral-angle violations [i](#)

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 |
| PHI | 85 | 50.0 | 23 | 27.1 | 13.5 | 0 | 0.0 | 0.0 |
| PSI | 85 | 50.0 | 34 | 40.0 | 20.0 | 0 | 0.0 | 0.0 |
| Total | 170 | 100.0 | 57 | 33.5 | 33.5 | 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](#)



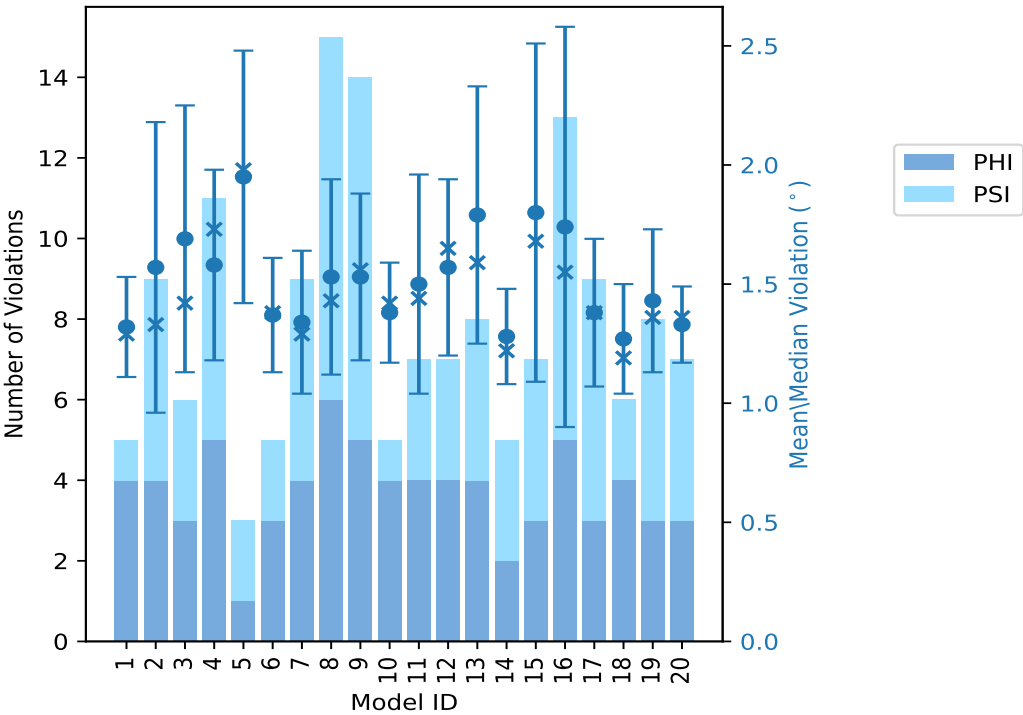
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PHI | PSI | Total | | | | |
| 1 | 4 | 1 | 5 | 1.32 | 1.65 | 0.21 | 1.29 |
| 2 | 4 | 5 | 9 | 1.57 | 3.13 | 0.61 | 1.33 |
| 3 | 3 | 3 | 6 | 1.69 | 2.79 | 0.56 | 1.42 |
| 4 | 5 | 6 | 11 | 1.58 | 2.15 | 0.4 | 1.73 |
| 5 | 1 | 2 | 3 | 1.95 | 2.58 | 0.53 | 1.98 |
| 6 | 3 | 2 | 5 | 1.37 | 1.79 | 0.24 | 1.38 |
| 7 | 4 | 5 | 9 | 1.34 | 2.07 | 0.3 | 1.29 |
| 8 | 6 | 9 | 15 | 1.53 | 2.4 | 0.41 | 1.43 |
| 9 | 5 | 9 | 14 | 1.53 | 2.23 | 0.35 | 1.56 |
| 10 | 4 | 1 | 5 | 1.38 | 1.7 | 0.21 | 1.42 |
| 11 | 4 | 3 | 7 | 1.5 | 2.51 | 0.46 | 1.44 |
| 12 | 4 | 3 | 7 | 1.57 | 2.14 | 0.37 | 1.65 |
| 13 | 4 | 4 | 8 | 1.79 | 2.79 | 0.54 | 1.59 |
| 14 | 2 | 3 | 5 | 1.28 | 1.58 | 0.2 | 1.22 |
| 15 | 3 | 4 | 7 | 1.8 | 3.07 | 0.71 | 1.68 |
| 16 | 5 | 8 | 13 | 1.74 | 3.8 | 0.84 | 1.55 |
| 17 | 3 | 6 | 9 | 1.38 | 2.11 | 0.31 | 1.38 |
| 18 | 4 | 2 | 6 | 1.27 | 1.72 | 0.23 | 1.19 |
| 19 | 3 | 5 | 8 | 1.43 | 2.03 | 0.3 | 1.36 |
| 20 | 3 | 4 | 7 | 1.33 | 1.52 | 0.16 | 1.36 |

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 | |
|-------------------------------|-----|-------|--------------------------|------|
| PHI | PSI | Total | Count ¹ | % |
| 9 | 17 | 26 | 1 | 5.0 |
| 3 | 8 | 11 | 2 | 10.0 |
| 1 | 3 | 4 | 3 | 15.0 |
| 3 | 0 | 3 | 4 | 20.0 |
| 4 | 3 | 7 | 5 | 25.0 |
| 2 | 0 | 2 | 6 | 30.0 |
| 0 | 0 | 0 | 7 | 35.0 |
| 0 | 1 | 1 | 8 | 40.0 |
| 0 | 1 | 1 | 9 | 45.0 |
| 0 | 0 | 0 | 10 | 50.0 |
| 0 | 1 | 1 | 11 | 55.0 |

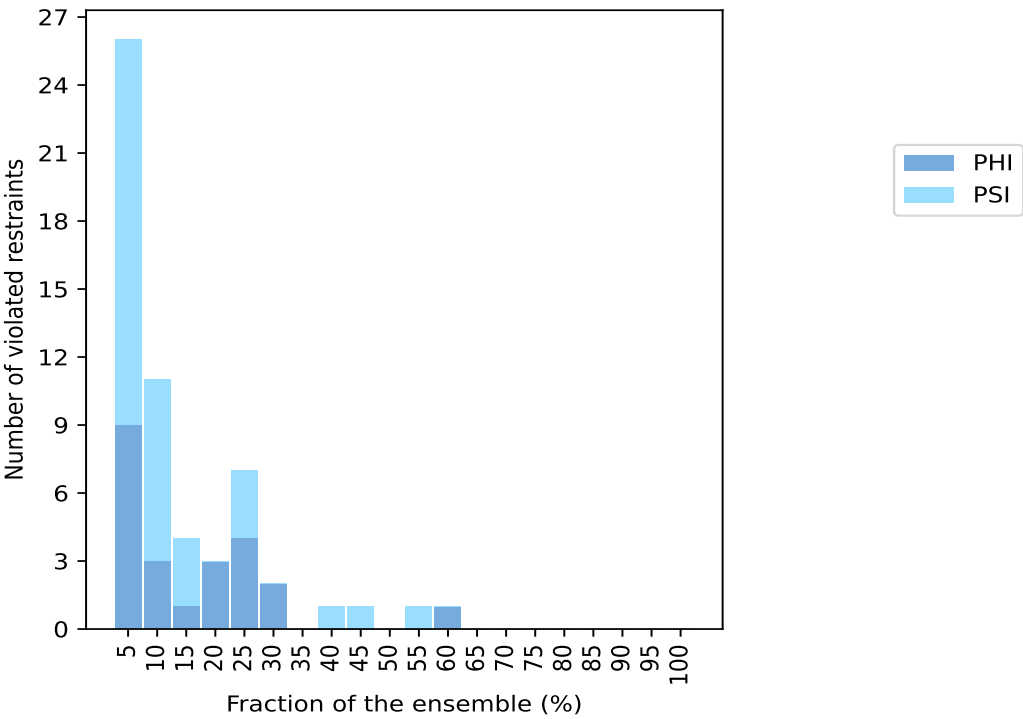
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI | PSI | Total | Count ¹ | % |
| 1 | 0 | 1 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 | 0 | 14 | 70.0 |
| 0 | 0 | 0 | 15 | 75.0 |
| 0 | 0 | 0 | 16 | 80.0 |
| 0 | 0 | 0 | 17 | 85.0 |
| 0 | 0 | 0 | 18 | 90.0 |
| 0 | 0 | 0 | 19 | 95.0 |
| 0 | 0 | 0 | 20 | 100.0 |

¹ Number of models with violations

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

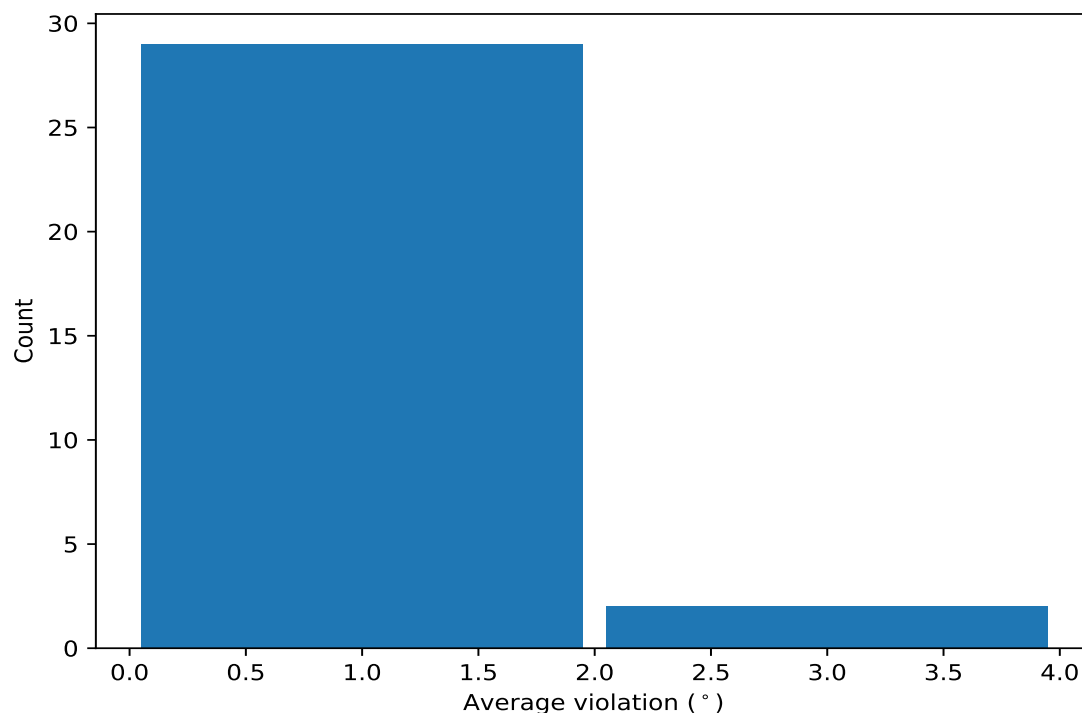


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|--------------|---------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 12 | 1.68 | 0.44 | 1.48 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 11 | 1.77 | 0.6 | 1.58 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 9 | 1.63 | 0.58 | 1.47 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 8 | 1.68 | 0.26 | 1.63 |
| (1,45) | 1:34:A:ARG:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 6 | 2.02 | 0.93 | 1.62 |
| (1,101) | 1:67:A:GLU:C | 1:68:A:VAL:N | 1:68:A:VAL:CA | 1:68:A:VAL:C | 6 | 1.28 | 0.15 | 1.31 |
| (1,82) | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 1:55:A:HIS:N | 5 | 1.59 | 0.53 | 1.39 |
| (1,153) | 1:98:A:GLU:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 5 | 1.58 | 0.44 | 1.56 |
| (1,113) | 1:73:A:GLY:C | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C | 5 | 1.46 | 0.35 | 1.43 |
| (1,148) | 1:95:A:ASP:N | 1:95:A:ASP:CA | 1:95:A:ASP:C | 1:96:A:GLY:N | 5 | 1.45 | 0.22 | 1.35 |
| (1,61) | 1:43:A:ARG:C | 1:44:A:HIS:N | 1:44:A:HIS:CA | 1:44:A:HIS:C | 5 | 1.37 | 0.43 | 1.05 |
| (1,81) | 1:53:A:ASP:C | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 5 | 1.31 | 0.11 | 1.27 |
| (1,74) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C | 1:51:A:VAL:N | 5 | 1.14 | 0.12 | 1.17 |
| (1,49) | 1:36:A:VAL:C | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 4 | 1.62 | 0.17 | 1.62 |
| (1,79) | 1:52:A:GLN:C | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 4 | 1.59 | 0.3 | 1.56 |
| (1,41) | 1:32:A:ALA:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 4 | 1.52 | 0.25 | 1.6 |
| (1,47) | 1:35:A:LEU:C | 1:36:A:VAL:N | 1:36:A:VAL:CA | 1:36:A:VAL:C | 3 | 1.98 | 0.35 | 1.91 |
| (1,154) | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 1:100:A:THR:N | 3 | 1.42 | 0.14 | 1.49 |
| (1,80) | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 1:54:A:ASP:N | 3 | 1.28 | 0.14 | 1.3 |
| (1,50) | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 1:38:A:VAL:N | 3 | 1.18 | 0.06 | 1.21 |

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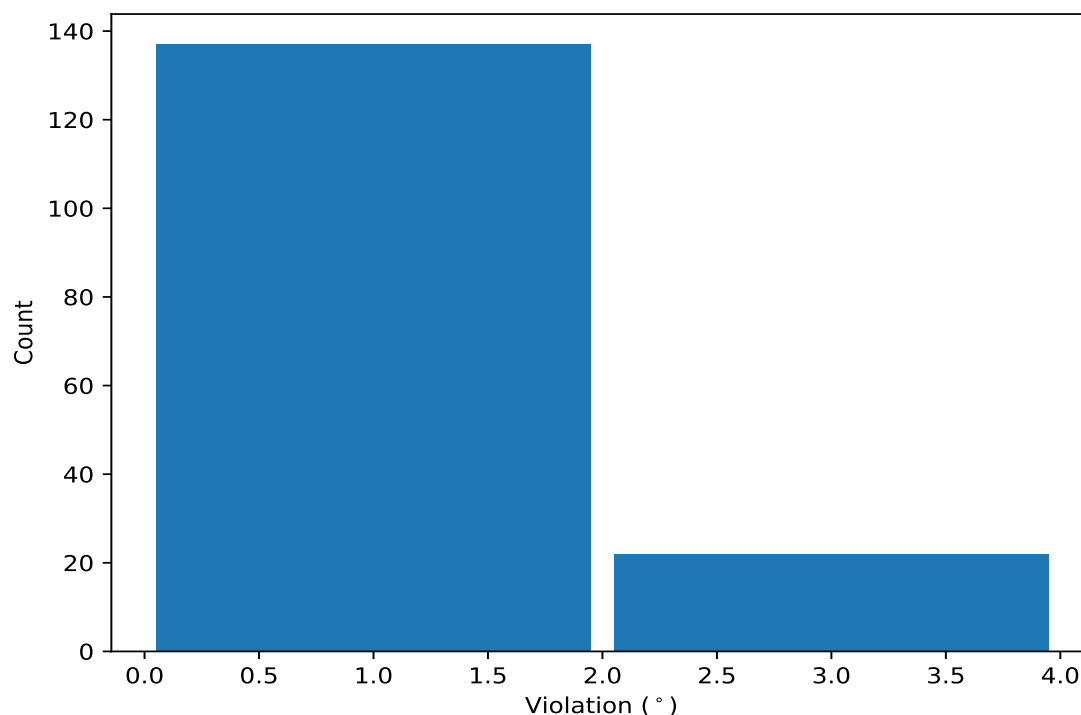
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,44) | 1:34:A:ARG:N | 1:34:A:ARG:CA | 1:34:A:ARG:C | 1:35:A:LEU:N | 2 | 2.62 | 1.18 | 2.62 |
| (1,48) | 1:36:A:VAL:N | 1:36:A:VAL:CA | 1:36:A:VAL:C | 1:37:A:LYS:N | 2 | 1.59 | 0.25 | 1.59 |
| (1,8) | 1:12:A:VAL:N | 1:12:A:VAL:CA | 1:12:A:VAL:C | 1:13:A:GLY:N | 2 | 1.59 | 0.52 | 1.59 |
| (1,16) | 1:17:A:SER:N | 1:17:A:SER:CA | 1:17:A:SER:C | 1:18:A:ALA:N | 2 | 1.45 | 0.18 | 1.45 |
| (1,20) | 1:19:A:LYS:N | 1:19:A:LYS:CA | 1:19:A:LYS:C | 1:20:A:TYR:N | 2 | 1.42 | 0.01 | 1.42 |
| (1,67) | 1:46:A:SER:C | 1:47:A:SER:N | 1:47:A:SER:CA | 1:47:A:SER:C | 2 | 1.41 | 0.36 | 1.41 |
| (1,110) | 1:72:A:ASP:N | 1:72:A:ASP:CA | 1:72:A:ASP:C | 1:73:A:GLY:N | 2 | 1.34 | 0.04 | 1.34 |
| (1,35) | 1:29:A:ILE:C | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C | 2 | 1.18 | 0.1 | 1.18 |
| (1,100) | 1:67:A:GLU:N | 1:67:A:GLU:CA | 1:67:A:GLU:C | 1:68:A:VAL:N | 2 | 1.15 | 0.06 | 1.15 |
| (1,7) | 1:11:A:THR:C | 1:12:A:VAL:N | 1:12:A:VAL:CA | 1:12:A:VAL:C | 2 | 1.12 | 0.01 | 1.12 |
| (1,72) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:GLU:N | 2 | 1.11 | 0.01 | 1.11 |

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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,44) | 1:34:A:ARG:N | 1:34:A:ARG:CA | 1:34:A:ARG:C | 1:35:A:LEU:N | 16 | 3.8 |
| (1,45) | 1:34:A:ARG:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 16 | 3.38 |
| (1,45) | 1:34:A:ARG:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 2 | 3.13 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 15 | 3.07 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 3 | 2.79 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 13 | 2.79 |
| (1,82) | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 1:55:A:HIS:N | 5 | 2.58 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 11 | 2.51 |
| (1,47) | 1:35:A:LEU:C | 1:36:A:VAL:N | 1:36:A:VAL:CA | 1:36:A:VAL:C | 13 | 2.45 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 8 | 2.4 |
| (1,62) | 1:44:A:HIS:N | 1:44:A:HIS:CA | 1:44:A:HIS:C | 1:45:A:ASP:N | 15 | 2.38 |
| (1,153) | 1:98:A:GLU:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 8 | 2.35 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 9 | 2.23 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 4 | 2.15 |
| (1,165) | 1:104:A:SER:C | 1:105:A:SER:N | 1:105:A:SER:CA | 1:105:A:SER:C | 12 | 2.14 |
| (1,63) | 1:44:A:HIS:C | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 15 | 2.14 |
| (1,8) | 1:12:A:VAL:N | 1:12:A:VAL:CA | 1:12:A:VAL:C | 1:13:A:GLY:N | 17 | 2.11 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 7 | 2.07 |
| (1,45) | 1:34:A:ARG:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 3 | 2.05 |
| (1,79) | 1:52:A:GLN:C | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 19 | 2.03 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 4 | 2.01 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 13 | 2.0 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 5 | 1.98 |
| (1,113) | 1:73:A:GLY:C | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C | 9 | 1.98 |
| (1,61) | 1:43:A:ARG:C | 1:44:A:HIS:N | 1:44:A:HIS:CA | 1:44:A:HIS:C | 4 | 1.97 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 2 | 1.94 |
| (1,47) | 1:35:A:LEU:C | 1:36:A:VAL:N | 1:36:A:VAL:CA | 1:36:A:VAL:C | 12 | 1.91 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 9 | 1.88 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 16 | 1.87 |
| (1,114) | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C | 1:75:A:TYR:N | 4 | 1.86 |
| (1,48) | 1:36:A:VAL:N | 1:36:A:VAL:CA | 1:36:A:VAL:C | 1:37:A:LYS:N | 8 | 1.84 |
| (1,49) | 1:36:A:VAL:C | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 9 | 1.82 |
| (1,61) | 1:43:A:ARG:C | 1:44:A:HIS:N | 1:44:A:HIS:CA | 1:44:A:HIS:C | 16 | 1.8 |
| (1,148) | 1:95:A:ASP:N | 1:95:A:ASP:CA | 1:95:A:ASP:C | 1:96:A:GLY:N | 6 | 1.79 |
| (1,41) | 1:32:A:ALA:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 4 | 1.79 |
| (1,67) | 1:46:A:SER:C | 1:47:A:SER:N | 1:47:A:SER:CA | 1:47:A:SER:C | 8 | 1.77 |
| (1,113) | 1:73:A:GLY:C | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C | 4 | 1.73 |
| (1,49) | 1:36:A:VAL:C | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 13 | 1.73 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 18 | 1.72 |
| (1,54) | 1:39:A:LYS:N | 1:39:A:LYS:CA | 1:39:A:LYS:C | 1:40:A:VAL:N | 19 | 1.72 |
| (1,164) | 1:104:A:SER:N | 1:104:A:SER:CA | 1:104:A:SER:C | 1:105:A:SER:N | 12 | 1.71 |
| (1,79) | 1:52:A:GLN:C | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 10 | 1.7 |
| (1,153) | 1:98:A:GLU:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 15 | 1.68 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 8 | 1.68 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 12 | 1.65 |
| (1,41) | 1:32:A:ALA:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 1 | 1.65 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 8 | 1.64 |
| (1,60) | 1:43:A:ARG:N | 1:43:A:ARG:CA | 1:43:A:ARG:C | 1:44:A:HIS:N | 16 | 1.63 |
| (1,16) | 1:17:A:SER:N | 1:17:A:SER:CA | 1:17:A:SER:C | 1:18:A:ALA:N | 9 | 1.63 |
| (1,148) | 1:95:A:ASP:N | 1:95:A:ASP:CA | 1:95:A:ASP:C | 1:96:A:GLY:N | 11 | 1.62 |
| (1,82) | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 1:55:A:HIS:N | 7 | 1.59 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,47) | 1:35:A:LEU:C | 1:36:A:VAL:N | 1:36:A:VAL:CA | 1:36:A:VAL:C | 9 | 1.59 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 9 | 1.58 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 17 | 1.58 |
| (1,38) | 1:31:A:THR:N | 1:31:A:THR:CA | 1:31:A:THR:C | 1:32:A:ALA:N | 14 | 1.58 |
| (1,162) | 1:103:A:ARG:N | 1:103:A:ARG:CA | 1:103:A:ARG:C | 1:104:A:SER:N | 2 | 1.57 |
| (1,153) | 1:98:A:GLU:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 16 | 1.56 |
| (1,154) | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 1:100:A:THR:N | 16 | 1.55 |
| (1,42) | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 1:34:A:ARG:N | 9 | 1.55 |
| (1,41) | 1:32:A:ALA:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 11 | 1.55 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 20 | 1.52 |
| (1,49) | 1:36:A:VAL:C | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 2 | 1.52 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 16 | 1.51 |
| (1,81) | 1:53:A:ASP:C | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 20 | 1.51 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 19 | 1.51 |
| (1,154) | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 1:100:A:THR:N | 3 | 1.49 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 10 | 1.47 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 20 | 1.47 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 19 | 1.46 |
| (1,77) | 1:51:A:VAL:C | 1:52:A:GLN:N | 1:52:A:GLN:CA | 1:52:A:GLN:C | 13 | 1.45 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 8 | 1.44 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 13 | 1.44 |
| (1,101) | 1:67:A:GLU:C | 1:68:A:VAL:N | 1:68:A:VAL:CA | 1:68:A:VAL:C | 14 | 1.44 |
| (1,80) | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 1:54:A:ASP:N | 17 | 1.44 |
| (1,44) | 1:34:A:ARG:N | 1:34:A:ARG:CA | 1:34:A:ARG:C | 1:35:A:LEU:N | 11 | 1.44 |
| (1,113) | 1:73:A:GLY:C | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C | 8 | 1.43 |
| (1,20) | 1:19:A:LYS:N | 1:19:A:LYS:CA | 1:19:A:LYS:C | 1:20:A:TYR:N | 8 | 1.43 |
| (1,101) | 1:67:A:GLU:C | 1:68:A:VAL:N | 1:68:A:VAL:CA | 1:68:A:VAL:C | 10 | 1.42 |
| (1,79) | 1:52:A:GLN:C | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 12 | 1.42 |
| (1,20) | 1:19:A:LYS:N | 1:19:A:LYS:CA | 1:19:A:LYS:C | 1:20:A:TYR:N | 9 | 1.42 |
| (1,131) | 1:82:A:LYS:C | 1:83:A:LEU:N | 1:83:A:LEU:CA | 1:83:A:LEU:C | 18 | 1.41 |
| (1,101) | 1:67:A:GLU:C | 1:68:A:VAL:N | 1:68:A:VAL:CA | 1:68:A:VAL:C | 17 | 1.41 |
| (1,82) | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 1:55:A:HIS:N | 1 | 1.39 |
| (1,49) | 1:36:A:VAL:C | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 6 | 1.39 |
| (1,110) | 1:72:A:ASP:N | 1:72:A:ASP:CA | 1:72:A:ASP:C | 1:73:A:GLY:N | 17 | 1.38 |
| (1,75) | 1:50:A:GLU:C | 1:51:A:VAL:N | 1:51:A:VAL:CA | 1:51:A:VAL:C | 6 | 1.38 |
| (1,82) | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 1:55:A:HIS:N | 20 | 1.36 |
| (1,148) | 1:95:A:ASP:N | 1:95:A:ASP:CA | 1:95:A:ASP:C | 1:96:A:GLY:N | 4 | 1.35 |
| (1,81) | 1:53:A:ASP:C | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 7 | 1.34 |
| (1,48) | 1:36:A:VAL:N | 1:36:A:VAL:CA | 1:36:A:VAL:C | 1:37:A:LYS:N | 3 | 1.34 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 2 | 1.33 |
| (1,46) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:VAL:N | 13 | 1.32 |
| (1,110) | 1:72:A:ASP:N | 1:72:A:ASP:CA | 1:72:A:ASP:C | 1:73:A:GLY:N | 2 | 1.3 |
| (1,80) | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 1:54:A:ASP:N | 7 | 1.3 |
| (1,74) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C | 1:51:A:VAL:N | 9 | 1.3 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 7 | 1.29 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 3 | 1.29 |
| (1,148) | 1:95:A:ASP:N | 1:95:A:ASP:CA | 1:95:A:ASP:C | 1:96:A:GLY:N | 5 | 1.29 |
| (1,64) | 1:45:A:ASP:N | 1:45:A:ASP:CA | 1:45:A:ASP:C | 1:46:A:SER:N | 11 | 1.29 |
| (1,35) | 1:29:A:ILE:C | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C | 1 | 1.29 |
| (1,81) | 1:53:A:ASP:C | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 1 | 1.27 |
| (1,16) | 1:17:A:SER:N | 1:17:A:SER:CA | 1:17:A:SER:C | 1:18:A:ALA:N | 19 | 1.27 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|---------------|----------|---------------|
| (1,136) | 1:88:A:TRP:N | 1:88:A:TRP:CA | 1:88:A:TRP:C | 1:89:A:TYR:N | 8 | 1.26 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 19 | 1.24 |
| (1,81) | 1:53:A:ASP:C | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 17 | 1.23 |
| (1,79) | 1:52:A:GLN:C | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 2 | 1.23 |
| (1,50) | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 1:38:A:VAL:N | 16 | 1.23 |
| (1,154) | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 1:100:A:THR:N | 8 | 1.22 |
| (1,81) | 1:53:A:ASP:C | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 14 | 1.22 |
| (1,74) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C | 1:51:A:VAL:N | 20 | 1.22 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 15 | 1.21 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 18 | 1.21 |
| (1,101) | 1:67:A:GLU:C | 1:68:A:VAL:N | 1:68:A:VAL:CA | 1:68:A:VAL:C | 4 | 1.21 |
| (1,100) | 1:67:A:GLU:N | 1:67:A:GLU:CA | 1:67:A:GLU:C | 1:68:A:VAL:N | 8 | 1.21 |
| (1,50) | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 1:38:A:VAL:N | 8 | 1.21 |
| (1,153) | 1:98:A:GLU:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 3 | 1.2 |
| (1,45) | 1:34:A:ARG:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 7 | 1.2 |
| (1,148) | 1:95:A:ASP:N | 1:95:A:ASP:CA | 1:95:A:ASP:C | 1:96:A:GLY:N | 9 | 1.19 |
| (1,149) | 1:96:A:GLY:C | 1:97:A:ASP:N | 1:97:A:ASP:CA | 1:97:A:ASP:C | 6 | 1.18 |
| (1,45) | 1:34:A:ARG:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 18 | 1.18 |
| (1,74) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C | 1:51:A:VAL:N | 4 | 1.17 |
| (1,45) | 1:34:A:ARG:C | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 10 | 1.17 |
| (1,130) | 1:82:A:LYS:N | 1:82:A:LYS:CA | 1:82:A:LYS:C | 1:83:A:LEU:N | 13 | 1.15 |
| (1,101) | 1:67:A:GLU:C | 1:68:A:VAL:N | 1:68:A:VAL:CA | 1:68:A:VAL:C | 20 | 1.14 |
| (1,96) | 1:65:A:ILE:N | 1:65:A:ILE:CA | 1:65:A:ILE:C | 1:66:A:VAL:N | 17 | 1.13 |
| (1,9) | 1:13:A:GLY:C | 1:14:A:THR:N | 1:14:A:THR:CA | 1:14:A:THR:C | 10 | 1.13 |
| (1,7) | 1:11:A:THR:C | 1:12:A:VAL:N | 1:12:A:VAL:CA | 1:12:A:VAL:C | 19 | 1.13 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 15 | 1.12 |
| (1,72) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:GLU:N | 9 | 1.12 |
| (1,41) | 1:32:A:ALA:C | 1:33:A:LYS:N | 1:33:A:LYS:CA | 1:33:A:LYS:C | 16 | 1.11 |
| (1,116) | 1:75:A:TYR:N | 1:75:A:TYR:CA | 1:75:A:TYR:C | 1:76:A:GLN:N | 12 | 1.1 |
| (1,91) | 1:61:A:LYS:C | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C | 8 | 1.1 |
| (1,80) | 1:53:A:ASP:N | 1:53:A:ASP:CA | 1:53:A:ASP:C | 1:54:A:ASP:N | 20 | 1.1 |
| (1,72) | 1:49:A:VAL:N | 1:49:A:VAL:CA | 1:49:A:VAL:C | 1:50:A:GLU:N | 14 | 1.1 |
| (1,70) | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 1:49:A:VAL:N | 4 | 1.1 |
| (1,7) | 1:11:A:THR:C | 1:12:A:VAL:N | 1:12:A:VAL:CA | 1:12:A:VAL:C | 18 | 1.1 |
| (1,153) | 1:98:A:GLU:C | 1:99:A:LYS:N | 1:99:A:LYS:CA | 1:99:A:LYS:C | 19 | 1.09 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 2 | 1.09 |
| (1,115) | 1:74:A:ALA:C | 1:75:A:TYR:N | 1:75:A:TYR:CA | 1:75:A:TYR:C | 7 | 1.09 |
| (1,113) | 1:73:A:GLY:C | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C | 11 | 1.09 |
| (1,100) | 1:67:A:GLU:N | 1:67:A:GLU:CA | 1:67:A:GLU:C | 1:68:A:VAL:N | 6 | 1.09 |
| (1,50) | 1:37:A:LYS:N | 1:37:A:LYS:CA | 1:37:A:LYS:C | 1:38:A:VAL:N | 9 | 1.09 |
| (1,113) | 1:73:A:GLY:C | 1:74:A:ALA:N | 1:74:A:ALA:CA | 1:74:A:ALA:C | 7 | 1.08 |
| (1,35) | 1:29:A:ILE:C | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C | 12 | 1.08 |
| (1,140) | 1:90:A:THR:N | 1:90:A:THR:CA | 1:90:A:THR:C | 1:91:A:VAL:N | 7 | 1.07 |
| (1,92) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C | 1:63:A:GLY:N | 16 | 1.07 |
| (1,84) | 1:55:A:HIS:N | 1:55:A:HIS:CA | 1:55:A:HIS:C | 1:56:A:ILE:N | 16 | 1.07 |
| (1,8) | 1:12:A:VAL:N | 1:12:A:VAL:CA | 1:12:A:VAL:C | 1:13:A:GLY:N | 14 | 1.07 |
| (1,152) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C | 1:99:A:LYS:N | 17 | 1.05 |
| (1,101) | 1:67:A:GLU:C | 1:68:A:VAL:N | 1:68:A:VAL:CA | 1:68:A:VAL:C | 16 | 1.05 |
| (1,67) | 1:46:A:SER:C | 1:47:A:SER:N | 1:47:A:SER:CA | 1:47:A:SER:C | 9 | 1.05 |
| (1,61) | 1:43:A:ARG:C | 1:44:A:HIS:N | 1:44:A:HIS:CA | 1:44:A:HIS:C | 17 | 1.05 |
| (1,82) | 1:54:A:ASP:N | 1:54:A:ASP:CA | 1:54:A:ASP:C | 1:55:A:HIS:N | 2 | 1.01 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,74) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C | 1:51:A:VAL:N | 15 | 1.01 |
| (1,74) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C | 1:51:A:VAL:N | 18 | 1.01 |
| (1,61) | 1:43:A:ARG:C | 1:44:A:HIS:N | 1:44:A:HIS:CA | 1:44:A:HIS:C | 1 | 1.01 |
| (1,61) | 1:43:A:ARG:C | 1:44:A:HIS:N | 1:44:A:HIS:CA | 1:44:A:HIS:C | 8 | 1.01 |
| (1,39) | 1:31:A:THR:C | 1:32:A:ALA:N | 1:32:A:ALA:CA | 1:32:A:ALA:C | 11 | 1.01 |
| (1,30) | 1:26:A:GLU:N | 1:26:A:GLU:CA | 1:26:A:GLU:C | 1:27:A:ALA:N | 4 | 1.0 |